**S2 Table. The fragment peaks of detected peptides in M451**

**Table A the fragment peaks of peptide GAGAGAGY**

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **b⁺** | **b-H₂O⁺** | **b-NH₃⁺** | **Seq.** | **y-H₂O⁺** | **y-NH₃⁺** | **y⁺** |
| 58.02875 | 40.01818 | 41.00220 | G |  |  |  |
| 129.06587 | 111.05530 | 112.03932 | A | 548.24637 | 549.23038 | 566.25693 |
| 186.08734 | 168.07677 | 169.06079 | G | 477.20925 | 478.19326 | 495.21981 |
| 257.12446 | 239.11389 | 240.09791 | A | 420.18778 | 421.17179 | 438.19834 |
| 314.14593 | 296.13536 | 297.11938 | G | 349.15066 | 350.13467 | 367.16122 |
| 385.18305 | 367.17248 | 368.15650 | A | 292.12919 | 293.11320 | 310.13975 |
| 442.20452 | 424.19395 | 425.17797 | G | 221.09207 | 222.07608 | 239.10263 |
|  |  |  | Y | 164.07060 | 165.05461 | 182.08116 |

**Table B the fragment peaks of peptide GAGVGAGY**

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **b⁺** | **b-H₂O⁺** | **b-NH₃⁺** | **Seq.** | **y-H₂O⁺** | **y-NH₃⁺** | **y⁺** |
| 58.02875 | 40.01818 | 41.00220 | G |  |  |  |
| 129.06587 | 111.05530 | 112.03932 | A | 576.27767 | 577.26168 | 594.28823 |
| 186.08734 | 168.07677 | 169.06079 | G | 505.24055 | 506.22456 | 523.25111 |
| 285.15576 | 267.14519 | 268.12921 | V | 448.21908 | 449.20309 | 466.22964 |
| 342.17723 | 324.16666 | 325.15068 | G | 349.15066 | 350.13467 | 367.16122 |
| 413.21435 | 395.20378 | 396.18780 | A | 292.12919 | 293.11320 | 310.13975 |
| 470.23582 | 452.22525 | 453.20927 | G | 221.09207 | 222.07608 | 239.10263 |
|  |  |  | Y | 164.07060 | 165.05461 | 182.08116 |

**Table C the fragment peaks of peptide GAGAGSGAGSGAGAGSGAGAGY**

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **b⁺** | **b²⁺** | **b-H₂O⁺** | **b-H₂O²⁺** | **b-NH₃⁺** | **b-NH₃²⁺** | **Seq.** | **y-H₂O⁺** | **y-H₂O²⁺** | **y-NH₃⁺** | **y-NH₃²⁺** | **y⁺** | **y²⁺** |
| 58.02875 | 29.51801 | 40.01818 | 20.51273 | 41.00220 | 21.00474 | G |  |  |  |  |  |  |
| 129.06587 | 65.03657 | 111.05530 | 56.03129 | 112.03932 | 56.52330 | A | 1492.64123 | 746.82425 | 1493.62524 | 747.31626 | 1510.65179 | 755.82953 |
| 186.08734 | 93.54731 | 168.07677 | 84.54202 | 169.06079 | 85.03403 | G | 1421.60411 | 711.30569 | 1422.58812 | 711.79770 | 1439.61467 | 720.31097 |
| 257.12446 | 129.06587 | 239.11389 | 120.06058 | 240.09791 | 120.55259 | A | 1364.58264 | 682.79496 | 1365.56665 | 683.28696 | 1382.59320 | 691.80024 |
| 314.14593 | 157.57660 | 296.13536 | 148.57132 | 297.11938 | 149.06333 | G | 1293.54552 | 647.27640 | 1294.52953 | 647.76840 | 1311.55608 | 656.28168 |
| 401.17796 | 201.09262 | 383.16739 | 192.08733 | 384.15141 | 192.57934 | S | 1236.52405 | 618.76566 | 1237.50806 | 619.25767 | 1254.53461 | 627.77094 |
| 458.19943 | 229.60335 | 440.18886 | 220.59807 | 441.17288 | 221.09008 | G | 1149.49202 | 575.24965 | 1150.47603 | 575.74165 | 1167.50258 | 584.25493 |
| 529.23655 | 265.12191 | 511.22598 | 256.11663 | 512.21000 | 256.60864 | A | 1092.47055 | 546.73891 | 1093.45456 | 547.23092 | 1110.48111 | 555.74419 |
| 586.25802 | 293.63265 | 568.24745 | 284.62736 | 569.23147 | 285.11937 | G | 1021.43343 | 511.22035 | 1022.41744 | 511.71236 | 1039.44399 | 520.22563 |
| 673.29005 | 337.14866 | 655.27948 | 328.14338 | 656.26350 | 328.63539 | S | 964.41196 | 482.70962 | 965.39597 | 483.20162 | 982.42252 | 491.71490 |
| 730.31152 | 365.65940 | 712.30095 | 356.65411 | 713.28497 | 357.14612 | G | 877.37993 | 439.19360 | 878.36394 | 439.68561 | 895.39049 | 448.19888 |
| 801.34864 | 401.17796 | 783.33807 | 392.17267 | 784.32209 | 392.66468 | A | 820.35846 | 410.68287 | 821.34247 | 411.17487 | 838.36902 | 419.68815 |
| 858.37011 | 429.68869 | 840.35954 | 420.68341 | 841.34356 | 421.17542 | G | 749.32134 | 375.16431 | 750.30535 | 375.65631 | 767.33190 | 384.16959 |
| 929.40723 | 465.20725 | 911.39666 | 456.20197 | 912.38068 | 456.69398 | A | 692.29987 | 346.65357 | 693.28388 | 347.14558 | 710.31043 | 355.65885 |
| 986.42870 | 493.71799 | 968.41813 | 484.71270 | 969.40215 | 485.20471 | G | 621.26275 | 311.13501 | 622.24676 | 311.62702 | 639.27331 | 320.14029 |
| 1073.46073 | 537.23400 | 1055.45016 | 528.22872 | 1056.43418 | 528.72073 | S | 564.24128 | 282.62428 | 565.22529 | 283.11628 | 582.25184 | 291.62956 |
| 1130.48220 | 565.74474 | 1112.47163 | 556.73945 | 1113.45565 | 557.23146 | G | 477.20925 | 239.10826 | 478.19326 | 239.60027 | 495.21981 | 248.11354 |
| 1201.51932 | 601.26330 | 1183.50875 | 592.25801 | 1184.49277 | 592.75002 | A | 420.18778 | 210.59753 | 421.17179 | 211.08953 | 438.19834 | 219.60281 |
| 1258.54079 | 629.77403 | 1240.53022 | 620.76875 | 1241.51424 | 621.26076 | G | 349.15066 | 175.07897 | 350.13467 | 175.57097 | 367.16122 | 184.08425 |
| 1329.57791 | 665.29259 | 1311.56734 | 656.28731 | 1312.55136 | 656.77932 | A | 292.12919 | 146.56823 | 293.11320 | 147.06024 | 310.13975 | 155.57351 |
| 1386.59938 | 693.80333 | 1368.58881 | 684.79804 | 1369.57283 | 685.29005 | G | 221.09207 | 111.04967 | 222.07608 | 111.54168 | 239.10263 | 120.05495 |
|  |  |  |  |  |  | Y | 164.07060 | 82.53894 | 165.05461 | 83.03094 | 182.08116 | 91.54422 |

**Table D the fragment peaks of peptide GAGAGSGAASGAGAGAGAGAGTGSSGF**

|  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **b⁺** | **b²⁺** | **b-H₂O⁺** | **b-H₂O²⁺** | **b-NH₃⁺** | **b-NH₃²⁺** | **Seq.** | **y-H₂O⁺** | **y-H₂O²⁺** | **y-NH₃⁺** | **y-NH₃²⁺** | **y⁺** | **y²⁺** |
| 58.02875 | 29.51801 | 40.01818 | 20.51273 | 41.00220 | 21.00474 | G |  |  |  |  |  |  |
| 129.06587 | 65.03657 | 111.05530 | 56.03129 | 112.03932 | 56.52330 | A | 1863.82175 | 932.41451 | 1864.80576 | 932.90652 | 1881.83231 | 941.41979 |
| 186.08734 | 93.54731 | 168.07677 | 84.54202 | 169.06079 | 85.03403 | G | 1792.78463 | 896.89595 | 1793.76864 | 897.38796 | 1810.79519 | 905.90123 |
| 257.12446 | 129.06587 | 239.11389 | 120.06058 | 240.09791 | 120.55259 | A | 1735.76316 | 868.38522 | 1736.74717 | 868.87722 | 1753.77372 | 877.39050 |
| 314.14593 | 157.57660 | 296.13536 | 148.57132 | 297.11938 | 149.06333 | G | 1664.72604 | 832.86666 | 1665.71005 | 833.35866 | 1682.73660 | 841.87194 |
| 401.17796 | 201.09262 | 383.16739 | 192.08733 | 384.15141 | 192.57934 | S | 1607.70457 | 804.35592 | 1608.68858 | 804.84793 | 1625.71513 | 813.36120 |
| 458.19943 | 229.60335 | 440.18886 | 220.59807 | 441.17288 | 221.09008 | G | 1520.67254 | 760.83991 | 1521.65655 | 761.33191 | 1538.68310 | 769.84519 |
| 529.23655 | 265.12191 | 511.22598 | 256.11663 | 512.21000 | 256.60864 | A | 1463.65107 | 732.32917 | 1464.63508 | 732.82118 | 1481.66163 | 741.33445 |
| 600.27367 | 300.64047 | 582.26310 | 291.63519 | 583.24712 | 292.12720 | A | 1392.61395 | 696.81061 | 1393.59796 | 697.30262 | 1410.62451 | 705.81589 |
| 687.30570 | 344.15649 | 669.29513 | 335.15120 | 670.27915 | 335.64321 | S | 1321.57683 | 661.29205 | 1322.56084 | 661.78406 | 1339.58739 | 670.29733 |
| 744.32717 | 372.66722 | 726.31660 | 363.66194 | 727.30062 | 364.15395 | G | 1234.54480 | 617.77604 | 1235.52881 | 618.26804 | 1252.55536 | 626.78132 |
| 815.36429 | 408.18578 | 797.35372 | 399.18050 | 798.33774 | 399.67251 | A | 1177.52333 | 589.26530 | 1178.50734 | 589.75731 | 1195.53389 | 598.27058 |
| 872.38576 | 436.69652 | 854.37519 | 427.69123 | 855.35921 | 428.18324 | G | 1106.48621 | 553.74674 | 1107.47022 | 554.23875 | 1124.49677 | 562.75202 |
| 943.42288 | 472.21508 | 925.41231 | 463.20979 | 926.39633 | 463.70180 | A | 1049.46474 | 525.23601 | 1050.44875 | 525.72801 | 1067.47530 | 534.24129 |
| 1000.44435 | 500.72581 | 982.43378 | 491.72053 | 983.41780 | 492.21254 | G | 978.42762 | 489.71745 | 979.41163 | 490.20945 | 996.43818 | 498.72273 |
| 1071.48147 | 536.24437 | 1053.47090 | 527.23909 | 1054.45492 | 527.73110 | A | 921.40615 | 461.20671 | 922.39016 | 461.69872 | 939.41671 | 470.21199 |
| 1128.50294 | 564.75511 | 1110.49237 | 555.74982 | 1111.47639 | 556.24183 | G | 850.36903 | 425.68815 | 851.35304 | 426.18016 | 868.37959 | 434.69343 |
| 1199.54006 | 600.27367 | 1181.52949 | 591.26838 | 1182.51351 | 591.76039 | A | 793.34756 | 397.17742 | 794.33157 | 397.66942 | 811.35812 | 406.18270 |
| 1256.56153 | 628.78440 | 1238.55096 | 619.77912 | 1239.53498 | 620.27113 | G | 722.31044 | 361.65886 | 723.29445 | 362.15086 | 740.32100 | 370.66414 |
| 1327.59865 | 664.30296 | 1309.58808 | 655.29768 | 1310.57210 | 655.78969 | A | 665.28897 | 333.14812 | 666.27298 | 333.64013 | 683.29953 | 342.15340 |
| 1384.62012 | 692.81370 | 1366.60955 | 683.80841 | 1367.59357 | 684.30042 | G | 594.25185 | 297.62956 | 595.23586 | 298.12157 | 612.26241 | 306.63484 |
| 1485.66780 | 743.33754 | 1467.65723 | 734.33225 | 1468.64125 | 734.82426 | T | 537.23038 | 269.11883 | 538.21439 | 269.61083 | 555.24094 | 278.12411 |
| 1542.68927 | 771.84827 | 1524.67870 | 762.84299 | 1525.66272 | 763.33500 | G | 436.18270 | 218.59499 | 437.16671 | 219.08699 | 454.19326 | 227.60027 |
| 1629.72130 | 815.36429 | 1611.71073 | 806.35900 | 1612.69475 | 806.85101 | S | 379.16123 | 190.08425 | 380.14524 | 190.57626 | 397.17179 | 199.08953 |
| 1716.75333 | 858.88030 | 1698.74276 | 849.87502 | 1699.72678 | 850.36703 | S | 292.12920 | 146.56824 | 293.11321 | 147.06024 | 310.13976 | 155.57352 |
| 1773.77480 | 887.39104 | 1755.76423 | 878.38575 | 1756.74825 | 878.87776 | G | 205.09717 | 103.05222 | 206.08118 | 103.54423 | 223.10773 | 112.05750 |
|  |  |  |  |  |  | F | 148.07570 | 74.54149 | 149.05971 | 75.03349 | 166.08626 | 83.54677 |