Supplemental Information

Title

Rapid MRSA detection via tandem mass spectrometry of the intact 80kDa PBP2a

resistance protein

Authors

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Supplemental Table S1.

Observed wild-type PBP2a_{mecA} precursor ions during LC-separation and MS detection, associated charge states, and estimated intact protein masses (kDa).

| Precursor (m/z) | Charge State | Estimated Mass |
|-----------------|--------------|----------------|
| 749.0506 | 108 | 80789.46 |
| 756.0164 | 107 | 80786.75 |
| 763.1251 | 106 | 80785.26 |
| 770.4351 | 105 | 80790.69 |
| 777.7800 | 104 | 80785.12 |
| 785.3582 | 103 | 80788.89 |
| 793.0142 | 102 | 80785.45 |
| 800.8558 | 101 | 80785.44 |
| 808.8633 | 100 | 80786.33 |
| 817.0276 | 99 | 80786.73 |
| 825.3572 | 98 | 80787.01 |
| 833.8500 | 97 | 80786.45 |
| 842.5315 | 96 | 80787.02 |
| 851.3875 | 95 | 80786.81 |
| 860.4332 | 94 | 80786.72 |
| 869.6699 | 93 | 80786.30 |
| 879.1185 | 92 | 80786.90 |
| 888.8340 | 91 | 80792.89 |
| 898.6044 | 90 | 80784.40 |
| 908.6761 | 89 | 80783.17 |
| 919.0220 | 88 | 80785.94 |
| 929.5832 | 87 | 80786.74 |
| 940.3804 | 86 | 80786.71 |
| 951.4436 | 85 | 80787.71 |
| 962.7549 | 84 | 80787.41 |
| 974.3535 | 83 | 80788.34 |
| 986.1979 | 82 | 80786.23 |
| 998.3879 | 81 | 80788.42 |

Supplemental Table S2.

Observed recombinant His₆-PBP2a_{mecA} precursor ions during static infusion and MS detection, associated charge states, and estimated intact protein mass (kDa).

| Precursor (m/z) | Charge State | Estimated Mass |
|-----------------|--------------|----------------|
| 689.4417 | 110 | 75728.59 |
| 695.7183 | 109 | 75724.29 |
| 702.0076 | 108 | 75708.82 |
| 708.4284 | 107 | 75694.84 |
| 714.9862 | 106 | 75682.54 |
| 721.6894 | 105 | 75672.39 |
| 728.4697 | 104 | 75656.85 |
| 735.4249 | 103 | 75645.76 |
| 742.4749 | 102 | 75630.44 |
| 749.6928 | 101 | 75617.97 |
| 757.0309 | 100 | 75603.09 |
| 764.5173 | 99 | 75588.21 |
| 772.1490 | 98 | 75572.60 |
| 779.9485 | 97 | 75558.00 |
| 787.8883 | 96 | 75541.28 |
| 796.0026 | 95 | 75525.25 |
| 804.2679 | 94 | 75507.18 |
| 812.7720 | 93 | 75494.80 |
| 821.3775 | 92 | 75474.73 |
| 830.2002 | 91 | 75457.22 |
| 839.2721 | 90 | 75444.49 |
| 848.0000 | 89 | 75383.00 |
| 857.8789 | 88 | 75405.34 |
| 867.4464 | 87 | 75380.84 |
| 877.3149 | 86 | 75363.08 |
| 887.4195 | 85 | 75345.66 |
| 897.7188 | 84 | 75324.38 |
| 908.2631 | 83 | 75302.84 |
| 919.0792 | 82 | 75282.49 |
| 930.1249 | 81 | 75259.12 |
| 941.4857 | 80 | 75238.86 |
| 953.0951 | 79 | 75215.51 |
| 965.0383 | 78 | 75194.99 |
| 977.0000 | 77 | 75152.00 |
| 989.7187 | 76 | 75142.62 |

Supplemental Table S3.

Observed wild-type PBP2a_{mecA} precursor ions during chromatographic separation and charge-reduced using PTCR and MS detection approach, associated charge states, and estimated intact protein masses (kDa).

| Precursor (m/z) | Charge State | Estimated Mass |
|-----------------|--------------|----------------|
| 851.40 | 95 | 80788.00 |
| 860.50 | 94 | 80793.00 |
| 869.70 | 93 | 80789.10 |
| 879.10 | 92 | 80785.20 |
| 888.70 | 91 | 80780.70 |
| 898.50 | 90 | 80775.00 |
| 908.60 | 89 | 80776.40 |
| 919.00 | 88 | 80784.00 |
| 929.50 | 87 | 80779.50 |
| 940.20 | 86 | 80771.20 |
| 951.20 | 85 | 80767.00 |

Supplemental Table S4.

| Location | Protein Fragment | Amino Acids | Charge State | m/z (observed) | m/z (theoretical) | ∆m (ppm) |
|----------|---------------------|----------------|-----------------|----------------|-------------------|----------|
| | b ₉ | 1-9 | 2+ | 540.3544 | 540.3541 | 0.56 |
| | b 10 | 1-10 | 2+ | 596.8964 | 596.8961 | 0.50 |
| 10 | I - | 4.44 | 3+ | 435.9615 | 435.9612 | 0.69 |
| S, | D11 | 1-11 | 2+ | 653.4386 | 653.4382 | 0.61 |
| 1 | | 1.10 | 3+ | 473.6561 | 473.6559 | 0.42 |
| - | D 12 | 1-12 | 2+ | 709.9804 | 709.9802 | 0.28 |
| 3 | b13 | 1-13 | 3+ | 506.6790 | 506.6787 | 0.59 |
| Ĵ | | | 2+ | 759.5153 | 759.5144 | 1.18 |
| te | | | 3+ | 539.7018 | 539.7015 | 0.56 |
| - | D14 | 1-14 | 2+ | 809.0488 | 809.0486 | 0.25 |
| ~ | h | 4.45 | 3+ | 572.7245 | 572.7243 | 0.35 |
| | D ₁₅ | 1-15 | 2+ | 858.5835 | 858.5828 | 0.82 |
| | b ₁₆ | 1-16 | 3+ | 605.7474 | 605.7471 | 0.50 |
| | | | 16+ | 1011.0194 | 1011.0178 | 1.58 |
| | V 142 | 527-668 | 15+ | 1078.3536 | 1078.3519 | -1.67 |
| | , | | 14+ | 1155.3075 | 1155.3051 | 2.08 |
| | | 530-668 | 18+ | 881.5087 | 881.5074 | 1.47 |
| | | | 17+ | 933.3032 | 933.3016 | 1.71 |
| | y 139 | | 16+ | 991.5708 | 991.5699 | 0.91 |
| | | | 15+ | 1057.6087 | 1057.6075 | 1.13 |
| | | | 14+ | 1133.0804 | 1133.0789 | 1.32 |
| | | | 16+ | 969.4337 | 969.4308 | 2.99 |
| | y 136 | 533-668 | 15+ | 1033.9942 | 1033.9923 | 1.84 |
| S | - | | 14+ | 1107.7779 | 1107.7770 | 0.81 |
| 'n | y 134 | 534-668 | 17+ | 900.6949 | 900.6931 | 2.00 |
| Ū | | | 16+ | 956.9248 | 956.9235 | 1.36 |
| ir | | | 15+ | 1020.6525 | 1020.6513 | 1.18 |
| <u> </u> | | | 14+ | 1093.4859 | 1093.4830 | 2.65 |
| er | y 131 | 538-668 | 16+ | 936.8547 | 936.8527 | 2.13 |
| Ĕ | | | 15+ | 999.2422 | 999.2424 | -0.20 |
| | | | 14+ | 1070.5486 | 1070.5449 | 3.46 |
| 0 |) | 539-668 | 17+ | 875.1519 | 875.1510 | 1.03 |
| | | | 16+ | 929.7858 | 929.7850 | 0.86 |
| | y 130 | | 15+ | - | 991.7035 | - |
| | | | 14+ | 1062.4694 | 1062.4675 | 1.79 |
| | | 129 540-668 | 17+ | 867.5609 | 867.5602 | 0.81 |
| | y 129 | | 16+ | 921.7205 | 921.7198 | 0.76 |
| | | | 15+ | 983.1018 | 983.1006 | 1.22 |
| | | | 14+ | 1053.2520 | 1053.2502 | 1.71 |
| | y 127 | 542-668 | 16+ | 907.4661 | 907.4644 | 1.87 |
| | | | 15+ | 967.8971 | 967.8949 | 2.27 |
| | | | 14+ | 1036.9611 | 1036.9583 | 2.70 |

Observed wild-type PBP2a_{mecA} MS/MS product ions for precursor m/z 793.0 (charge state = 102) using HCD dissociation on a Q Exactive HF mass spectrometer.

Note: y_{130}^{15+} was not observed as isotopic pattern overlaps with y_{139}^{16+}

Supplemental Table S5.

Observed PBP2a_{mecA} peptides following cell lysate fractionation or in-gel digestion of immunopurified PBP2a from ATCC MRSA isolate BAA-44, associated charge states, observed and theoretical m/z values, mass error (ppm), and enzymes used.

| 2:26 KIKIVPLULVVVOFGIVPASK 3 88:38:0 3:2 Typ 34:40 DKEINTIDALEDK 2 609:402 809:401 4.1 Typ 34:44 IDALEDK 2 402:109 0 Prot K 48:54 DSSYISK 2 402:893 40:883 1.1 Prot K 55:68 SDNGEVEMTERPIK 2 402:897 47:2260 0.0 Typ 69:76 IYNSIGVK 2 447:286 47:2260 0.0 Typ 77:83 DINIOP 2 447:287 47:2261 1.8 Typ 101-110 RVDAQYK 2 440:237 1.1 Typ 101-111 NVGPNENR 2 440:237 1.8 Typ 111-118 NVGPNEVK 2 466:271 1.8 Typ 125-128 LDWOHSVIIPGMOK 3 464:462 440:461 2.1 Typ 124-229 KMDEYLSDFAK 3 464:564 46:564 46:564 <t< th=""><th>Location</th><th colspan="3">Location Sequence</th><th>m/z (theor.)</th><th>Error (ppm)</th><th>Enzyme</th></t<> | Location | Location Sequence | | | m/z (theor.) | Error (ppm) | Enzyme |
|---|----------|---|---|-----------|-----------------|----------------|--------|
| 27-40 DKEINNTIDALEDK 2 080-4019 4.1 Typ 34-44 IDAIEDK 2 002-109 402-109 0 Prot K 48-54 DSSYISK 2 400-1990 400-1991 1.7 Typ 55-68 SDNGEVEMTERPIK 2 402-2891 3.5 Typ 69-76 IYNLGCVK 2 447-2886 447-2886 0.3 Typ 94-100 RVDAQYK 2 447-2887 447-2886 1.8 Typ 94-100 RVDAQYK 2 447-2887 1.8 Typ 101-110 IKNYGNIDR 3 586-480 4.0 Typ 125-138 LDWDHSVIIPGMQK 3 586-480 4.0 Typ 213-241 FHLTTNETESR 3 440-5841 4.0 Typ 230-241 KHLTNETESR 3 445-5844 4.4 Typ 230-241 KHLTNETESR 3 445-5844 4.4 Typ 248-265 ATS | 2-26 | KIKIVPLILIVVVVGFGIYFYASK | 3 | 893.8949 | 893.8920 | 3.2 | Tryp |
| 34-40 IDALEDK 2 402:100 0 Prot K 34-44 IDALEDKKPKQ 3 440.8985 40.8985 1.1 Prot K 48-64 DSSYISK 2 40.9897 80.1985 7.7 Typ 55-68 SDNGEVEMTERPIK 2 40.2897 80.2802 3.5 Typ 69-76 IYNELGVK 2 447.2894 47.2822 0.3 Typ 77-83 DINIGDR 2 477.287 478.2747 1.8 Typ 101-110 IKTNYGNIDR 3 3086480 368.473 1.8 Typ 111-118 NVQFNFVK 2 488.271 4.8 Typ 125-138 LDWOHSVIPGMQK 3 546.801 54.8048 4.8 Typ 139-448 DQSIHENLK 3 309.5461 3.2 Typ 230-241 FFHLTTNETESR 3 449.5494 448.5441 42 Typ 248-265 ATSHLGYVGPINSEELK 3 649.3423 | 27-40 | 7-40 DKEINNTIDAIEDK | | | 809.4019 | 4.1 | Tryp |
| 34-44 IDAIEDKNFRQ 3 440888 1.1 Prot K 48-54 DSSYISK 2 4001980 4001893 3.5 Tryp 55-68 SDNGEVEMTERPIK 2 402.887 3.5 Tryp 77-83 DINIQDR 2 447.289 447.289 447.289 417.27 1.8 Tryp 94-100 RVDAOYK 2 447.289 440.281 410.221 1.8 Tryp 94-101 IKTNYGNIDR 2 447.287 1.8 Tryp 103-110 IKTNYGNIDR 2 447.287 4.8 4.0 Tryp 125-138 LDWOHSVIIPGMOK 3 564.801 4.0 Tryp 213-241 FMLTTNETESR 3 446.5644 4.2 Tryp 231-241 FMLTTNETESR 3 445.5044 4.8 Tryp 248-265 ATSHLIGYVGPINSEELK 3 583.2842 3.8 1.6 Tryp 230-241 FMLTTNETESR 3 445.50 | 34-40 | IDAIEDK | | 402.2109 | 402.2109 | 0 | Prot K |
| 48-54 DSSYISK 2 400.198.3 1.7 Tryp 55-68 SDNGEVEMTERPIK 2 902.897 902.893 1.5 Tryp 69-76 INNSLGVK 2 447.292 0.8 Tryp 94-100 RVDAQYK 2 447.292 440.2376 1.1 Tryp 94-100 RVDAQYK 2 440.2376 1.1 Tryp 101-110 IKTNYGNDR 3 366.460 366.473 1.8 Tryp 103-110 TNYGNDR 2 446.274 446.277 1.8 Tryp 111-118 NVQFNFVK 2 488.281 4.0 Tryp 125-138 LDWDHSVIIPGMCK 3 346.840 2.1 Tryp 219-229 KMDEYLSDFAK 3 449.5481 4.0 Tryp 230-241 KFHLTTNETESR 3 449.5481 2.2 Tryp 231-241 FHLTTNETESR 3 442.5284 4.8 Tryp 246.265 | 34-44 | IDAIEDKNFKQ | 3 | 440.8985 | 440.8980 | 1.1 | Prot K |
| 55-68 SDNGEVEMTERPIK 2 802.829 3.5 Typ 69-76 NYNSLGVK 2 447.256 447.258 447.258 447.258 447.258 447.258 447.258 447.258 447.258 447.258 447.258 440.278 1.8 Typ 94-100 RVDAQYK 2 447.258 447.278 1.8 Typ 103-110 TNYGNIDR 2 447.278 1.8 Typ 125-138 LDWOHSVIFCKK 2 448.271 489.281 4.0 Tryp 230-241 KFHLTNETESR 3 449.544 489.271 5.6 Typ 230-241 KFHLTNETESR 3 446.5584 445.5584 4.2 Typ 231-241 FHLTINETESR 3 446.5584 445.5584 445.5584 445.5584 445.5584 445.5584 445.5584 445.5584 445.5584 445.5584 445.5584 445.5584 445.5584 445.5584 445.5584 445.5584 445.5584 445.5584 44 | 48-54 | DSSYISK | 2 | 400.1960 | 400.1953 | 1.7 | Tryp |
| 69-76 IYNSLGVK 2 447.252 67.252 67.92 77-83 DINIODR 2 437.227 437.229 61.8 Tryp 101-110 IKTNYGNIDR 3 388.440 388.4473 1.8 Tryp 101-110 IKTNYGNIDR 2 447.728 476.727 1.8 Tryp 111-118 NVOENPKK 2 448.247 488.2473 1.8 Tryp 125-138 LDWOHNEWIPEMOK 3 544.9510 548.9461 0.2 Tryp 139-148 DOSIHIENLK 3 399.5482 448.2471 488.2471 448.2471 488.2471 488.241 Tryp 248-265 ATTSHUCYCIPINSEKKK | 55-68 | SDNGEVEMTERPIK | 2 | 802.8857 | 802.8829 | 3.5 | Tryp |
| 77-83 DINIODR 2 4472.282 449.232 449.232 449.232 449.232 449.232 449.232 449.232 449.232 449.232 449.232 449.232 449.232 449.232 449.231 1.8 Typ 103-110 TNYGNIDR 2 448.271 486.271 1.8 Typ 103-110 TNYGNIDR 2 448.271 486.271 1.8 Typ 113-118 NVQFNFVK 2 448.271 486.271 5.6 Typ 125-138 LDWDHSVIJFORMCK 3 546.945 4.6 Typ 230-241 KFHLTTNETESR 3 448.247 486.247 0.6 Typ 231-241 FHLTTNETESR 3 448.544 482.241 6 Typ 248-265 ATSHLGYVGPINSEELK 3 845.231 6.3 Typ 230-241 KHUTENETESR 3 845.231 6.6 Prot K 293-300 GYKDDAVIGK 2 533.2842 3.3 | 69-76 | IYNSLGVK | 2 | 447.2586 | 447.2582 | 0.9 | Tryp |
| 94-100 RVDAQYK 2 440.2378 1.1 Trip 101-110 IKTNYGNIDR 3 998.548 368.473 1.8 Trip 111-118 NVQFNEVK 2 496.728 1.8 Trip 111-118 NVQFNEVK 2 498.2011 488.2014 4.0 Trip 125-138 LUWDHSVIPGMGK 3 546.8046 4.6 Trip 219-229 KMDEYLSDFAK 3 448.2041 488.2071 -0.6 Trip 231-241 FHLTINETESR 3 448.2044 488.2071 -0.6 Trip 231-241 FHLTINETESR 3 448.2044 42.2 Trip 248-265 ATSHLLGYVGPINSEELK 2 533.284 3.4 Trip 290-298 KLOHEOGYR 3 382.5281 463.323 1.6 Trip 230-31 DOKOLQUTDAK 3 843.974 1.1 Trip 301.11 IVDONSITIAH 2 598.7886 0.3 Prork K | 77-83 | DINIQDR | 2 | 437.2257 | 437.2249 | 1.8 | Tryp |
| 101-110 IKTNYGNIDR 3 398-8470 398-8470 18. Tryp 103-110 TNYGNIDR 2 476-728 476-7278 18. Tryp 111-118 NVQFNFVK 2 486-2011 <t< td=""><td>94-100</td><td>RVDAQYK</td><td>2</td><td>440.2382</td><td>440.2378</td><td>1.1</td><td>Tryp</td></t<> | 94-100 | RVDAQYK | 2 | 440.2382 | 440.2378 | 1.1 | Tryp |
| 110 TNYGNIDR 2 475.278 476.278 18. Typ 111-118 NVOFNEVK 2 498.2711 498.2811 4.0 Tryp 135-138 LDWDHSVIIPGMQK 3 546.546 366 Tryp 139-148 DQSIHIENLK 3 309.5468 389.472 3.5 Tryp 230-241 KFHLTINETESR 3 448.2474 488.2477 -0.6 Tryp 231-241 FHLTINETESR 3 448.5464 -2.2 Tryp 230-298 KLDHEDGYR 3 382.5281 -0.3 Tryp 290-298 KLDHEDGYR 3 382.5281 -0.3 Tryp 293-316 VTNDDNSITIAH 2 599.786 0.3 Prot K 320-331 DCKDQLTIDAK 3 439.5734 413.733 1.6 Prot K 332-331 DLQLTIDAK 3 493.5734 457.33 1.6 Prot K 332-3331 DLQLTIDAK 3 493.5734 1.1 | 101-110 | IKTNYGNIDR | 3 | 398.5480 | 398.5473 | 1.8 | Tryp |
| 111-118 NVQFNFVK 2 249-2711 498-2891 4.0 Tryp 125-138 LDWDHSVIIPGMQK 3 546.8485 4.6 Tryp 139-148 DQSIHIENLK 3 396.5482 3.6 Tryp 219-229 KMDEYLSDFAK 3 448.5482 445.5461 0.2 Tryp 230-241 KFHLTTINETESR 3 448.2477 0.6 Tryp 231-241 FHLTTNETESR 3 445.5004 445.5494 2.2 Tryp 248-265 ATSHILGYVOPINSEELK 3 643.3432 1.6 Tryp 290-298 KLOHEOGYR 3 382.5280 382.5281 -0.3 Tryp 293-300 HEDCYRVT 2 488.7271 0.6 Prot K 293-311 IVDDNSNTIAHTUEK 3 689.7886 0.3 Prot K 320-331 DGKDIOLTIDAK 3 439.5734 1.1 Tryp 322-331 DGKDIOLTIDAK 2 599.7886 0.8 1.6 < | 103-110 | TNYGNIDR | 2 | 476.7287 | 476.7278 | 1.8 | Tryp |
| 125-138 LDWDHSVIPGMOK 3 5 469.950 546.9485 4.6 Tryp 139-148 DQSIHIENLK 3 399.5486 399.5472 3.5 Tryp 219-229 KMDEYLSDFAK 3 449.5481 0.2 Tryp 230-241 KFHLTINETESR 3 449.5494 482.2477 0.6 Tryp 231-241 FHLTINETESR 3 445.5044 445.5494 2.2 Tryp 248-265 ATSHLGYVOPINSEELK 3 643.3432 1.6 Tryp 290-298 KLOHEDGYR 3 382.5281 0.3 Tryp 293.300 HEDGYRYT 2 489.7281 489.728 0.6 Prot K 301-311 IVDDNSNTIAH 2 599.788 599.7886 0.3 Prot K 320-331 DGKDIDIDAK 3 449.5734 1.1 Tryp 342-382 NDYGSGTAIHPOTGELLALVSTPSYDVPFMYGMSNEEYNK 3 159.744 1.1 Tryp 376-383 SNEEYNKL 2 | 111-118 | NVQFNFVK | 2 | 498.2711 | 498.2691 | 4.0 | Tryp |
| 139-148 DQSIHIENLK 3 3995486 3985472 3.5 Tryp 219-229 KMDEYLSDFAK 3 448.942 448.941 0.2 Tryp 230-241 KFHLTTNETESR 3 448.542 448.247 0.6 Tryp 231-241 FHLTTNETESR 3 445.504 445.544 2.2 Tryp 248-265 ATSHLIGYVOPINSEELK 3 643.343 443.423 1.6 Tryp 290-208 KLOHEOGYR 3 382.5280 382.5281 -0.3 Tryp 293-300 HEDGYRVT 2 488.7278 0.6 Prot K 293-301 DIGKDIOLTIDAK 3 498.5734 438.5734 438.5734 438.5734 301-311 IVDDNSNTIAH 2 599.7886 0.3 Prot K 320-331 DGKDIOLTIDAK 3 498.5734 438.5734 438.574 1.1 Tryp 376-383 SNEEYNKL 2 498.744 0.6 Tryp 376-383 | 125-138 | LDWDHSVIIPGMQK | 3 | 546.9510 | 546.9485 | 4.6 | Tryp |
| 219-229 KMDEYLSDFAK 3 449.5481 0.2 Tryp 230-241 KFHLTINETESR 3 449.5481 0.6 Tryp 231-241 FHLTINETESR 3 446.5401 446.5441 2.8 Tryp 248-265 ATSHLGYVGPINSEELK 3 446.5504 445.5444 2.8 7.7 248-265 ATSHLGYVGPINSEELK 3 482.5281 43.3 1.6 Tryp 290-298 KLQHEDGYR 3 382.5281 -0.3 Tryp 293-300 HEDGYRVT 2 488.7271 0.6 Prot K 299-316 VTIVDDNSNTIAHTLIEK 3 661.5646 2.1 Tryp 301-311 IVDDNSNTIAH 2 599.7886 0.3 Prot K 320-331 DIQLTIDAK 3 439.5731 439.574 1.1 Tryp 323-334 DIQLTIDAK 2 406.731 439.744 1.1 Tryp 332-394 LTEDKKEPLLNK 3 476.008 476.008 | 139-148 | DQSIHIENLK | 3 | 399.5486 | 399.5472 | 3.5 | Tryp |
| 230-241 KFHLTTNETESR 3 488.2477 488.2477 0.6 Typ 231-241 FHLTTNETESR 3 445.504 445.504 445.504 42.22 Typ 248-265 ATSHLLGYVGPINSEELK 3 643.333 643.333 643.333 643.333 643.333 643.333 643.333 643.333 643.333 643.333 643.332 643.333 643.333 643.333 643.333 643.233 643.233 643.233 643.233 643.233 643.233 643.243 643.243 643.243 643.243 643.243 643.243 643.243 643.243 643.243 643.243 704 704.733 704.743 704.743.733.736 704.733.7433.7433 704.74 | 219-229 | KMDEYLSDFAK | 3 | 449.5482 | 449.5481 | 0.2 | Tryp |
| 231-241 FHLTTNETESR 3 445.5504 445.5494 2.2 Typ 248-265 ATSHLLGYVGPINSEELK 3 643.3433 643.3423 1.6 Typ 271-280 GYKDDAVIGK 2 633.242 533.2824 3.4 Tryp 290-298 KLOHEDGYR 3 382.5280 382.5281 0.3 Tryp 293-300 HEDGYRVT 2 488.7281 488.728 0.6 Prot K 299-316 VTIVDDINSNTIAHTLIEK 3 661.6860 521.3613 35. Tryp 342.332 NDYGSGTAIHPQTGELLALVSTPSVDYPFMYGMSNEEYNK 3 452.3660 12. Tryp | 230-241 | KFHLTTNETESR | 3 | 488.2474 | 488.2477 | -0.6 | Tryp |
| 248-265 ATSHLLGYVGPINSEELK 3 643.3433 643.3423 1.6 Typ 271-280 GYKDDAVIGK 2 633.2842 3.3 Typ 290-298 KLOHEDGYR 3 382.5280 382.2821 0.3 Tryp 293-300 HEDGYRVT 2 488.7281 488.7281 0.6 Prot K 299-316 VTIVDDNSNTIAHTLIEK 3 661.6860 661.6866 61 Tryp 301-311 IVDDNSNTIAH 2 699.7886 69.7886 60.3 Prot K 323-331 DGKDQLTIDAK 3 439.5734 1.1 Tryp 342-382 NDYGSGTAIHPQTGELLALVSTPSYDVYPFMYGMSNEEYNK 3 1521.3661 1521.3613 3.5 Tryp 335-406 FQITTSPGSTOK 2 647.8361 647.8355 0.9 Tryp 335-406 FQITTSPGSTOK 2 647.8361 647.8355 0.9 Tryp 407-417 ILTAMIGLNNK 2 602.3432 602.3432 0.3 Tryp </td <td>231-241</td> <td>FHI TTNETESR</td> <td>3</td> <td>445.5504</td> <td>445.5494</td> <td>2.2</td> <td>Tryp</td> | 231-241 | FHI TTNETESR | 3 | 445.5504 | 445.5494 | 2.2 | Tryp |
| 271-280 GYKDDAVIGK 2 533.2843 533.2812 533.2812 533.2812 533.2812 533.2812 533.281 633.281 633.281 633.281 633.281 633.283 533.281 633.283 533.281 633.283 77p 332-3394 LTEDKKEPLLNK 3 476.6083 3.22 Tryp 733.22 Tryp 734.233.283 <td>248-265</td> <td>ATSHI I GYVGPINSEELK</td> <td>3</td> <td>643,3433</td> <td>643.3423</td> <td>1.6</td> <td>Tryp</td> | 248-265 | ATSHI I GYVGPINSEELK | 3 | 643,3433 | 643.3423 | 1.6 | Tryp |
| 290-298 KLQHEDGYR 3 382.5280 382.5281 0.3 Tryp 293-300 HEDGYRVT 2 448.7271 0.6 Prot K 299-316 VTIVDDNSNTIAHTLIEK 3 661.8866 661.8866 0.3 Prot K 320-331 DGKDIQLTIDAK 3 439.5739 439.5734 1.1 Tryp 323-331 DIQLTIDAK 2 508.7861 508.7486 0.6 Fryp 342:382 NDYGSGTAIHPQTGELLALVSTPSYDVYPFMYGMSNEEYNK 3 1521.3066 1521.3613 3.5 Tryp 335:406 FQITTSPGSTQK 2 498.7381 498.7353 1.6 Prot K 407-417 ILTAMGLNNK 2 647.8361 647.8355 0.9 Tryp 418-426 TLDDKTSYK 3 357.5170 2.2 Tryp 446-456 YEVVNGNDLK 2 632.3326 0.3 Tryp 445-456 YEVNGNDLK 2 632.3326 0.3 Tryp 446-566 YEVNGNDLK </td <td>271-280</td> <td>GYKDDAVIGK</td> <td>2</td> <td>533.2842</td> <td>533.2824</td> <td>3.4</td> <td>Tryp</td> | 271-280 | GYKDDAVIGK | 2 | 533.2842 | 533.2824 | 3.4 | Tryp |
| 293-300 HEDGYRVT 2 488.7281 488.7278 0.6 Prof. K 293-300 VTIVDDNSNTIAHTLIEK 3 661.6864 2.1 Tryp 301-311 IVDDNSNTIAH 2 599.7888 509.7884 0.6 Tryp 320-331 DGKDIQLTIDAK 3 439.5734 1.1 Tryp 323-331 DIQCTIDAK 3 439.5734 40.6 Tryp 342-382 NDYGSGTAIHPQTGELLALVSTPSYDVYPEMYGMSNEEYNK 3 1521.3666 1521.3613 3.5 Tryp 376-383 SNEEYNKL 2 498.7361 498.7353 1.6 Prot K 335-406 FQITTSPGSTQK 2 647.3816 647.8355 0.3 Tryp 407-417 ILTAMIGLNNK 2 594.3447 594.3445 0.3 Tryp 407-417 ILTAMIGLNNK 2 602.3432 602.3419 2.2 Tryp 448.426 TLDDKTSYK 3 375.170 2.5 Tryp 435.445 DKSWGGYNVTR <td< td=""><td>290-298</td><td>KLQHEDGYR</td><td>3</td><td>382.5280</td><td>382.5281</td><td>-0.3</td><td>Tryp</td></td<> | 290-298 | KLQHEDGYR | 3 | 382.5280 | 382.5281 | -0.3 | Tryp |
| 209316 VTIVDDNSNTIAHTLIEK 3 661.6860 661.6866 2.1 Tryp 301-311 IVDDNSNTIAH 2 599.7886 599.7886 0.3 Prot K 320-331 DGKDIQLTIDAK 3 439.573 439.573 1.1 Tryp 323-331 DIQLTIDAK 2 508.7861 508.784 0.6 Tryp 323-331 DIQLTIDAK 2 498.7361 498.7353 1.6 Prot K 333-394 LTEDKKEPLLNK 3 476.608 498.7353 1.6 Prot K 333-394 LTEDKKEPLLNK 3 476.608 467.8355 0.9 Tryp 407-417 ILTAMIGLNNK 2 694.3447 594.3445 0.3 Tryp 407-417 ILTAMIGLNNK 2 602.342 602.342 602.342 0.3 Tryp 418-426 TLDDKTSYK 3 357.5179 357.5170 2.5 Tryp 446-456 YEVVNGNIDLK 2 602.3326 0.3 Tryp </td <td>293-300</td> <td>HEDGYRVT</td> <td>2</td> <td>488.7281</td> <td>488.7278</td> <td>0.6</td> <td>Prot K</td> | 293-300 | HEDGYRVT | 2 | 488.7281 | 488.7278 | 0.6 | Prot K |
| 20030 111 IVDDISINITIAH 2 599.786 0.3 Prot K 320-331 DGKDIQLTIDAK 3 439.5739 439.5734 1.1 Tryp 323-331 DIQLTIDAK 2 508.7861 508.784 0.6 Tryp 342-382 NDYGSGTAIHPQTGELLALVSTPSYDVYPFMYGMSNEEYNK 3 1521.3666 1521.3615 3.5 Tryp 376-383 SNEEYNKL 2 498.7361 498.7333 1.6 Prot K 335-406 FQITTSPCSTQK 2 647.8361 647.8365 0.9 Tryp 407-417 ILTAMIGLNNK 2 594.3447 594.3445 0.3 Tryp 407-417 ILTAMIGLNNK 2 602.3419 2.2 Tryp 418-426 TLDDKTSYK 3 357.517 395.5102 1.4 Tryp 446-456 YEVVNGNIDLK 2 632.328 603.3 Tryp 447-477 VALELGSK 2 749.3003 2.3 Tryp 4465-506 < | 299-316 | | 3 | 661,6860 | 661.6846 | 2.1 | Tryp |
| Solidit Tobolion 2 38,739 438,739 438,734 1.1 Tryp 320-331 DIQLTIDAK 2 508,784 1.1 Tryp 342-332 NDYGSGTAIHPQTGELLALVSTPSYDVYPFMYGMSNEEYNK 3 1521,3666 1521,3613 3.5 Tryp 376-383 SNEEYNKL 2 498,7361 498,7353 1.6 Prot K 383-394 LTEDKKEPLLNK 3 476,6098 476,6083 3.2 Tryp 395-406 FQITTSPGSTQK 2 647,8361 647,8355 0.9 Tryp 407-417 ILTAMIGLNNK 2 602,3447 594,3447 594,3445 0.3 Tryp 446-456 YEVVNGNIDLK 2 632,3326 0.3 Tryp 446-456 YEVVNGNIDLK 2 632,3326 0.3 Tryp 446-456 YEVVNGNIDLK 2 749,3700 749,3903 2.3 Tryp 446-456 YEVVNGNIDLK 2 762,786 776,3779 2.2 Tryp | 301-311 | IVDDNSNTIAH | 2 | 599.7888 | 599.7886 | 0.3 | Prot K |
| Bit State Dick Team Dick Team Dick Team Dick Team Typ 342-382 NDYGSGTAIHPQTGELLALVSTPSYDVYPFMYGMSNEEYNK 3 1521-3666 1521-3613 3.5 Tryp 376-383 SNEEYNKL 2 498.7361 498.7353 1.6 Prot K 383-394 LTEDKKEPLLNK 3 476.6098 476.6083 3.2 Tryp 395-406 FQITTSPGSTQK 2 647.8361 647.8355 0.9 Tryp 407-417 ILTAMIGLNNK 2 692.342 692.3449 2.2 Tryp 418-426 TLDDKTSYK 3 357.5170 2.5 Tryp 446-456 YEVVNGNIDLK 2 632.3326 0.3 Tryp 457-469 QAIESSDNIFFAR 2 749.3700 749.3903 2.3 Tryp 485-506 KLGVGEDIPSDYPFYNAQISNK 3 819.0778 819.0762 1.9 Tryp 505-513 NKNLDNEIL 2 566.7859 568.7853 1.1 Prot K | 320-331 | | 3 | 439 5739 | 439 5734 | 11 | Tryp |
| 342-382 NDYGSGTAIHPQTGELLALVSTPSYDVYPFMYGMSNEEYNK 3 1521-3666 1521-3616 1571-3613 3.5 Tryp 376-383 SNEEYNKL 2 498-7361 498-7353 1.6 Prot K 3394 LTEDKKEPLLNK 3 476-6084 476-6083 3.2 Tryp 407-417 ILTAMIGLNNK 2 647-8361 647-8356 0.9 Tryp 407-417 ILTAMIGLNNK 2 594-3447 594.3445 0.3 Tryp 435-445 DKSWGGYNVTR 3 367.5179 2.5 Tryp 446-456 YEVVNGNIDLK 2 632.3326 0.3 Tryp 446-456 YEVVNGNIDLK 2 632.3326 0.3 Tryp 446-456 YEVVNGNIDLK 2 408.7468 408.7493 2.2 Tryp 446-506 KLGVGEDIPSDYPFYNAQISNK 2 776.2766 776.3779 2.2 Tryp 486-506 KLGVGEDIPSDYPFYNAQISNK 2 776.2766 776.3779 2.2 Tryp <td>323-331</td> <td></td> <td>2</td> <td>508 7851</td> <td>508 7848</td> <td>0.6</td> <td>Tryp</td> | 323-331 | | 2 | 508 7851 | 508 7848 | 0.6 | Tryp |
| 376-383 SNEEYNKL 2 498.7361 498.7361 1.6 Prot K 383-394 LTEDKKEPILINK 3 476.6098 476.6098 476.6093 3.2 Tryp 395-406 FQITTSPGSTQK 2 647.8361 647.8355 0.9 Tryp 407-417 ILTAMIGLNNK 2 593.3447 594.3447 594.3445 0.3 Tryp 410-417 ILTAMIGLNNK 2 602.3422 602.3419 2.2 Tryp 418-426 TLDDKTSYK 3 357.5179 357.5170 2.5 Tryp 446-456 YEVVNGNIDLK 2 632.328 632.3326 0.3 Tryp 457-469 QAIESSDNIFFAR 2 749.3720 749.3903 2.3 Tryp 470-477 VALELGSK 2 408.7488 408.749 2.2 Tryp 485-506 LGVGEDIPSDYPFYNAQISNK 2 776.276 776.3779 2.2 Tryp 505-513 NKNLDNEIL 2 536.7853 <t< td=""><td>342-382</td><td></td><td>3</td><td>1521.3666</td><td>1521.3613</td><td>3.5</td><td>Tryp</td></t<> | 342-382 | | 3 | 1521.3666 | 1521.3613 | 3.5 | Tryp |
| Bit State Dirke Dirke Dirke Dirke Dirket 383-394 LTEDKKEPLLNK 3 476.6098 476.6083 3.2 Tryp 395-406 FQITTSPGSTQK 2 647.8361 647.8355 0.9 Tryp 407-417 ILTAMIGLNNK 2 594.3447 594.3445 0.3 Tryp 418-426 TLDDKTSYK 3 337.5179 357.5170 2.5 Tryp 435-445 DKSWGGYNVTR 3 428.2113 428.2107 1.4 Tryp 446-456 YEVVNGNIDLK 2 632.326 0.3 Tryp 470-477 VALELGSK 2 498.7458 408.7449 2.2 Tryp 485-506 KLGVGEDIPSDYPFYNAQISNK 2 776.3779 2.2 Tryp 507-551 NLDNEILLADSGYGQGEILINPVQILSIYSALENNGNINAPHLLK 3 1620.8566 1620.851 2.8 Tryp 582-589 THKEDIYR 3 364.5178 364.5173 1.4 Tryp 582- | 376-383 | SNEEYNKI | 2 | 498 7361 | 498 7353 | 1.6 | Prot K |
| Bit Direct Number Dire | 383-394 | | 3 | 476 6098 | 476 6083 | 32 | Tryp |
| 303 11/10 11/17 1 | 395-406 | 395-406 FQITTSPGSTQK | | 647 8361 | 647 8355 | 0.9 | Tryp |
| HOT HIT ILTAMIGLINIK ILTAMIGLINIK International constraints Int | 407-417 | 07-417 ILTAMIGLNNK | | 594 3447 | 594 3445 | 0.3 | Tryp |
| Hor Hill Linkinger Mit Lether Linkinger Mit Lether Hill Hill< Hill Hill | 407-417 | | 2 | 602 3432 | 602 3419 | 2.2 | Tryp |
| The Line Discrete | 418-426 | TI DDKTSYK | 3 | 357 5179 | 357 5170 | 2.5 | Tryp |
| Hose History Hose History< | 435-445 | 435-445 DKSWGGYNVTR | | 428 2113 | 428 2107 | 1.0 | Tryp |
| HO 400 Inclusion Important I | 446-456 | 446-456 YEV/NGNIDI K | | 632 3328 | 632 3326 | 0.3 | Tryp |
| 470-405 2 1433330 2.5 1133 470-477 VALELGSK 2 408.7458 408.7449 2.2 Tryp 485-506 KLGVGEDIPSDYPFYNAQISNK 3 819.0762 1.9 Tryp 505-513 NKNLDNEIL 2 536.7859 536.7853 1.1 Prot K 507-551 NLDNEILLADSGYGQGEILINPVQILSIYSALENNGNINAPHLLK 3 1620.8566 1620.8521 2.8 Tryp 582-589 THKEDIYR 3 354.5178 354.5173 1.4 Tryp 582-591 THKEDIYRSY 3 404.1998 404.1999 -0.2 Prot K 590-597 SYANLIGK 2 433.2442 433.2425 3.9 Tryp 613-634 QIGWFISYDKDNPNMMMAINVK 3 877.7516 877.7517 -0.1 Tryp 618-628 YDKDNPNMM 2 664.2878 664.2865 2.0 Prot K 620-628 YDKDNPNMM 2 564.224 482.6968 0.8 Prot K < | 457-469 | 440-450 TEVVINGNIDER 457-469 OAIESSDNIEEAP | | 749 3720 | 749 3903 | 23 | Tryp |
| HOLTITI VALEUSTYN 2 Holt HT 2 Tryp 505-513 LGVGEDIPSDYPFYNAQISNK 2 Tryp 2.2 Tryp 505-513 NKNLDNEIL 2 536.7859 536.7853 1.1 Prot K 507-551 NLDNEILLADSGYGQGEILINPVQILSIYSALENNGNINAPHLLK 3 1620.8566 1620.8521 2.8 Tryp 582-591 THKEDIYRSY 3 354.5178 354.5173 1.4 Tryp 583-591 HKEDIYRSY 3 404.1998 404.1999 -0.2 Prot K 590-597 SYANLIGK 2 433.2442 433.2425 3.9 Tryp 613-634 QIGWFISYDKDNPNMMMAINVK 3 877.751 | 470-477 | 457-469 QAIESSDNIFFAR | | 408 7458 | 408 7449 | 2.0 | Tryp |
| 486-506 LGVGEDIPSDYPFYNAQISNK 2 776.3779 2.2 Tryp 505-513 NKNLDNEIL 2 536.7859 536.7853 1.1 Prot K 507-551 NLDNEILLADSGYGQGEILINPVQILSIYSALENNGNINAPHLLK 3 1620.8566 1620.8521 2.8 Tryp 582-589 THKEDIYR 3 354.5178 354.5173 1.4 Tryp 582-591 THKEDIYRSY 3 404.1998 404.1999 -0.2 Prot K 590-597 SYANLIGK 2 353.1923 353.1925 3.9 Tryp 613-634 QIGWFISYDKDNPNmMMAINVK 3 877.7516 877.7517 -0.1 Tryp 613-628 ISYDKDNPNMM 2 664.2878 664.2865 2.0 Prot K 620-628 YDKDNPNMM 2 482.6972 482.6968 0.8 Prot K 621-628 DKDNPNMM 2 482.6972 482.6968 0.8 Prot K 620-628 YDKDNPNMM 2 482.6972 482.6968 0 | 485-506 | | | 819.0778 | 819.0762 | 1.0 | Тпур |
| Horizon Lovolution Lovolution <thlovolution< th=""> Lovolution Lovolution<</thlovolution<> | 486-506 | | | 776 2796 | 776 3779 | 22 | Tryp |
| 303-513 303-703 303-703 303-703 11.1 1101 R 507-551 NLDNEILLADSGYGQGEILINPVQILSIYSALENNGNINAPHLLK 3 1620.8566 1620.8521 2.8 Tryp 582-589 THKEDIYR 3 354.5178 354.5173 1.4 Tryp 582-591 THKEDIYRSY 3 404.1998 404.1999 -0.2 Prot K 583-591 HKEDIYRSY 3 437.8832 437.8824 1.8 Prot K 590-597 SYANLIGK 2 433.2442 433.2425 3.9 Tryp 598-604 SGTAELK 2 353.1923 353.1925 -0.6 Tryp 613-634 QIGWFISYDKDNPNMMMAINVK 3 877.7516 864.2865 2.0 Prot K 620-628 YDKDNPNMM 2 664.2878 664.2865 2.0 Prot K 621-628 DKDNPNMM 2 482.6972 482.6968 0.8 Prot K 640-647 GMASYNAK 2 421.1970 421.1973 -0.7 | 505-513 | | 2 | 536 7859 | 536 7853 | 1 1 | Prot K |
| 307-331 NEDNETEERDSOF OGGETEINIV ORIGIN GREENIVOONNALTHEER 3 1626.332 2.3 11yp 582-589 THKEDIYR 3 354.5178 354.5173 1.4 Tryp 582-591 THKEDIYRSY 3 404.1998 404.1999 -0.2 Prot K 583-591 HKEDIYRSY 3 437.8832 437.8824 1.8 Prot K 590-597 SYANLIGK 2 433.2442 433.2425 3.9 Tryp 598-604 SGTAELK 2 353.1923 353.1925 -0.6 Tryp 613-634 QIGWFISYDKDNPNMMMAINVK 3 877.7516 877.7517 -0.1 Tryp 613-628 ISYDKDNPNMM 2 664.2878 664.2864 2.0 Prot K 620-628 YDKDNPNMM 2 564.2294 564.2284 2.0 Prot K 621-628 DKDNPNMM 2 482.6972 482.6968 0.8 Prot K 640-647 GMASYNAK 2 421.1970 421.1973 -0.7 | 507-551 | | 2 | 1620 8566 | 1620 8521 | 2.8 | Tryp |
| 582-591 THKEDIYRSY 3 404.1998 404.1999 -0.2 Prot K 583-591 HKEDIYRSY 3 437.8832 437.8824 1.8 Prot K 583-591 HKEDIYRSY 3 437.8832 437.8824 1.8 Prot K 590-597 SYANLIGK 2 433.2442 433.2425 3.9 Tryp 598-604 SGTAELK 2 353.1923 353.1925 -0.6 Tryp 613-634 QIGWFISYDKDNPNmMMAINVK 3 877.7516 877.7517 -0.1 Tryp 613-628 ISYDKDNPNMM 2 664.2878 664.2865 2.0 Prot K 620-628 YDKDNPNMM 2 564.2294 564.2284 2.0 Prot K 621-628 DKDNPNMM 2 482.6972 482.6968 0.8 Prot K 640-647 GMASYNAK 2 421.1970 421.1973 -0.7 Tryp 652-662 VYDELYENGNK 2 672.3105 672.3093 1.8 | 582-589 | THKEDIYR | 3 | 354 5178 | 354 5173 | 1.0 | Ттур |
| 502 501 1111LEDTHOT 50 1011100 0.1 1011100 583-591 HKEDIYRSY 3 437.8832 437.8824 1.8 Prot K 590-597 SYANLIGK 2 433.2442 433.2425 3.9 Tryp 598-604 SGTAELK 2 353.1923 353.1925 -0.6 Tryp 613-634 QIGWFISYDKDNPNmMMAINVK 3 877.7516 877.7517 -0.1 Tryp 618-628 ISYDKDNPNMM 2 664.2878 664.2865 2.0 Prot K 620-628 YDKDNPNMM 2 564.2294 564.2284 2.0 Prot K 621-628 DKDNPNMM 2 482.6972 482.6968 0.8 Prot K 640-647 GMASYNAK 2 421.1970 421.1973 -0.7 Tryp 652-662 VYDELYENGNK 2 672.3105 672.3093 1.8 Tryp 663-668 KYDIDE 2 391.6818 391.6818 391.6820 -0.5 <td>582-591</td> <td>THKEDIYRSY</td> <td>3</td> <td>404 1998</td> <td>404 1999</td> <td>-0.2</td> <td>Prot K</td> | 582-591 | THKEDIYRSY | 3 | 404 1998 | 404 1999 | -0.2 | Prot K |
| 303-331 TREEDTRIST 3 437.3032 437.3032 1.0 1101 R 590-597 SYANLIGK 2 433.2442 433.2425 3.9 Tryp 598-604 SGTAELK 2 353.1923 353.1925 -0.6 Tryp 613-634 QIGWFISYDKDNPNmMMAINVK 3 877.7516 877.7517 -0.1 Tryp 618-628 ISYDKDNPNMM 2 664.2878 664.2865 2.0 Prot K 620-628 YDKDNPNMM 2 564.2874 564.2284 2.0 Prot K 621-628 DKDNPNMM 2 482.6972 482.6986 0.8 Prot K 640-647 GMASYNAK 2 421.1970 421.1973 -0.7 Tryp 652-662 VYDELYENGNK 2 672.3105 672.3093 1.8 Tryp 663-668 KYDIDE 2 391.6818 391.6818 Tryp | 583-501 | HKEDIYRSY | 3 | 437 8832 | 437 8824 | 1.8 | Prot K |
| 598-604 SGTAELK 2 460.24.0 60.3 11yp 598-604 SGTAELK 2 353.1923 353.1925 -0.6 Tryp 613-634 QIGWFISYDKDNPNmMMAINVK 3 877.7516 877.7517 -0.1 Tryp 613-628 ISYDKDNPNMM 2 664.2878 664.2865 2.0 Prot K 620-628 YDKDNPNMM 2 564.2294 564.2284 2.0 Prot K 621-628 DKDNPNMM 2 482.6972 482.6968 0.8 Prot K 640-647 GMASYNAK 2 421.1970 421.1973 -0.7 Tryp 652-662 VYDELYENGNK 2 672.3105 672.3093 1.8 Tryp 663-668 KYDIDE 2 391.6818 391.6820 -0.5 Tryp | 590-597 | SYANI IGK | 2 | 433 2442 | 433 2425 | 3.9 | Tryp |
| 613-634 QIGWFISYDKDNPNmMMAINVK 3 877.7516 877.7517 -0.1 Tryp 613-628 ISYDKDNPNmMMAINVK 3 877.7516 877.7517 -0.1 Tryp 613-628 ISYDKDNPNMM 2 664.2878 664.2865 2.0 Prot K 620-628 YDKDNPNMM 2 564.2294 564.2284 2.0 Prot K 621-628 DKDNPNMM 2 482.6972 482.6968 0.8 Prot K 640-647 GMASYNAK 2 421.1970 421.1973 -0.7 Tryp 652-662 VYDELYENGNK 2 672.3105 672.3093 1.8 Tryp 663-668 KYDIDE 2 391.6818 391.6820 -0.5 Tryp | 598-604 | SGTAFLK | 2 | 353 1923 | 353 1925 | -0.6 | Tryp |
| 613-628 ISYDKDNPNMM 2 664.2878 664.2865 2.0 Prot K 620-628 YDKDNPNMM 2 564.2294 564.2284 2.0 Prot K 621-628 DKDNPNMM 2 482.6972 482.6968 0.8 Prot K 621-628 DKDNPNMM 2 482.6972 482.6968 0.8 Prot K 640-647 GMASYNAK 2 421.1970 421.1973 -0.7 Tryp 652-662 VYDELYENGNK 2 672.3105 672.3093 1.8 Tryp 663-668 KYDIDE 2 391.6818 391.6818 391.6820 -0.5 Tryp | 613-634 | | 2 | 877 7516 | 877 7517 | -0.1 | Tryp |
| 610 620 101 DEDIterret Minimit 2 604.200 2.0 FIGUR 620-628 YDKDNPNMM 2 564.2294 564.2284 2.0 Prot K 621-628 DKDNPNMM 2 482.6972 482.6968 0.8 Prot K 640-647 GMASYNAK 2 421.1970 421.1973 -0.7 Tryp 652-662 VYDELYENGNK 2 672.3105 672.3093 1.8 Tryp 663-668 KYDIDE 2 391.6818 391.6820 -0.5 Tryp | 618-628 | | | 664 2878 | 664 2865 | 2.0 | Prot K |
| 620 620 1010101 2 301.2204 2.0 P101 K 621-628 DKDNPNMM 2 482.6968 0.8 Prot K 640-647 GMASYNAK 2 421.1970 421.1973 -0.7 Tryp 652-662 VYDELYENGNK 2 672.3105 672.3093 1.8 Tryp 663-668 KYDIDE 2 391.6818 391.6820 -0.5 Tryp | 620-628 | | | 564 22010 | 564 2284 | 2.0 | Prot K |
| 621-625 DRUNT INVITU 2 421.0900 0.5 FIGURE 640-647 GMASYNAK 2 421.1970 421.1973 -0.7 Tryp 652-662 VYDELYENGNK 2 672.3105 672.3093 1.8 Tryp 663-668 KYDIDE 2 391.6818 391.6820 -0.5 Tryp | 621-629 | | | 482 6972 | 482 6968 | 0.8 | Prot K |
| 652-662 VYDELYENGNK 2 672.3105 672.3093 1.8 Tryp 663-668 KYDIDE 2 391.6818 391.6820 -0.5 Tryp | 640-647 | | | 421 1070 | 421 1073 | -0.7 | |
| 663-668 KYDIDE 2 391.6818 391.6820 -0.5 Trvn | 652-662 | | 2 | 672 3105 | 672 3003 | 1.8 | Тпур |
| | 663-668 | | | 391,6818 | 391,6820 | -0.5 | Tryp |

Supplemental Table S6.

List of quality control and clinical MSSA and MRSA isolates, associated characteristics, and sources.

| Isolate | SCCmec | Resistance Gene | PFGE Type | Source | |
|-----------------------|-----------|--------------------|--------------|---|--|
| 12600 | - | - | n/a | American Type Culture Collection, USA | |
| 25923 | - | - | n/a | American Type Culture Collection, USA | |
| 29737 | - | - | n/a | American Type Culture Collection, USA | |
| BAA-44 | Type I | mecA | Iberian | American Type Culture Collection, USA | |
| BAA-41 | Type II | mecA | USA 100 | American Type Culture Collection, USA | |
| 33592 | Type III | mecA | ST239 | American Type Culture Collection, USA | |
| BAA-1683 | Type IV a | mecA | USA 400 | American Type Culture Collection, USA | |
| BAA-2094 | Type V | mecA | WA-MRSA | American Type Culture Collection, USA | |
| BAA-42 | Type VI | mecA | USA 800 | American Type Culture Collection, USA | |
| BAA-2313 | Type XI | mecC | CC130 | American Type Culture Collection, USA | |
| BAA-1761 | Type II | mecA | USA 100 | American Type Culture Collection, USA | |
| BAA-1720 | Type II | mecA | USA 200 | American Type Culture Collection, USA | |
| BAA-1717 | Type IV a | mecA | USA 300 | American Type Culture Collection, USA | |
| BAA-1707 | Type IV | mecA | USA 400 | American Type Culture Collection, USA | |
| BAA-1763 | Type IV | mecA | USA 500 | American Type Culture Collection, USA | |
| BAA-1754 | Type IV | mecA | USA 600 | American Type Culture Collection, USA | |
| BAA-1766 | Type V | mecA | USA 700 | American Type Culture Collection, USA | |
| BAA-1768 | Type IV | mecA | USA 800 | American Type Culture Collection, USA | |
| BAA-1747 | Type IV | mecA | USA 1000 | American Type Culture Collection, USA | |
| BAA-1764 | Type IV | mecA | USA 1100 | American Type Culture Collection, USA | |
| BAA-2312 | Type XI | mecC | n/a | American Type Culture Collection, USA | |
| BAA-42 | Type IV | mecA | USA 800 | American Type Culture Collection, USA | |
| 33591 | Type III | mecA | n/a | American Type Culture Collection, USA | |
| BAA-38 | Type I | mecA | n/a | American Type Culture Collection, USA | |
| BAA-1750 | Type II | mecA | USA 200 | American Type Culture Collection, USA | |
| BAA-1689 | Type IV | mecA | USA 500 | American Type Culture Collection, USA | |
| 43300 | Type II | mecA | n/a | American Type Culture Collection, USA | |
| BAA-1708 | Type II | mecA | n/a | American Type Culture Collection, USA | |
| MSSA Clin. Isolate 1 | - | - | n/a | St. George's University Hospital, London UK | |
| MRSA Clin. Isolate 1 | Type IV a | mecA | n/a | Univ. Hospital Ramón y Cajal, Madrid Spain | |
| MRSA Clin. Isolate 2 | n/a | mecA | n/a | Univ. Hospital Ramón y Cajal, Madrid Spain | |
| MRSA Clin. Isolate 3 | Type IV a | mecA | n/a | Univ. Hospital Ramón y Cajal, Madrid Spain | |
| MRSA Clin. Isolate 4 | n/a | mecA | n/a | Univ. Hospital Ramón y Cajal, Madrid Spain | |
| MRSA Clin. Isolate 5 | n/a | mecA | n/a | Univ. Hospital Ramón y Cajal, Madrid Spain | |
| MRSA Clin. Isolate 6 | Type IV a | mecA | n/a | Univ. Hospital Ramón y Cajal, Madrid Spain | |
| MRSA Clin. Isolate 7 | n/a | mecA | n/a | Univ. Hospital Ramón y Cajal, Madrid Spain | |
| MRSA Clin. Isolate 8 | n/a | mecA | n/a | Univ. Hospital Ramón y Cajal, Madrid Spain | |
| MRSA Clin. Isolate 9 | Type IV c | mecA | n/a | Univ. Hospital Ramón y Cajal, Madrid Spain | |
| MRSA Clin. Isolate 10 | Type IV c | mecA | n/a | Univ. Hospital Ramón y Cajal, Madrid Spain | |
| MRSA Clin. Isolate 11 | n/a | mecA | n/a | Univ. Hospital Ramón y Cajal, Madrid Spain | |
| MRSA Clin. Isolate 12 | Type IV a | mecA | n/a | Univ. Hospital Ramón y Cajal, Madrid Spain | |

n/a - not available

Supplemental Table S7.

N-terminal sequences from four different PBP2a variants, accession numbers, and species.

| PBP2a Variant | UniProt Accession Number | Species | N-terminal Sequence (15 amino acids) |
|-----------------------|-----------------------------|--------------------------|--|
| PBP2a _{mecA} | Q53707 | Staphylococcus aureus | MKKIKIVPLILIVVV |
| PBP2a _{mecB} | A0A4Y1NMT9 | Macrococcus canis | MKNKALAILIICICL |
| PBP2a _{mecC} | F4NA57 | Staphylococcus aureus | MKKIYISVLVLLLIM |
| PBP2a _{mecD} | A0A1S7BGS4 | Macrococcus caseolyticus | MKNIKVKILIVCSLC |

Intact recombinant His_6 -PBP2a_{mecA} MS/MS spectrum acquired with static infusion, isolation of precursor ion at m/z = 742.5, isolation window of 3 Th.



Detection of recombinant SDS-PAGE separated His_6 -PBP2a_{mecA} (1µg) and immunopurified PBP2a_{mecA} from ATCC MRSA isolate BAA-44 with ProQ Emerald glycoprotein stain, and total protein using Sypro Ruby total protein stain or silver stain (left side). Detection of immunopurified protein components before and after treatment with deglycosylation mix (right side). Original gel images are displayed on the next page.



Supplemental Figure S2. cont.

Below are the original gel images for the previous figure. Red boxes highlight those areas of the gel that have been selected for display.

20160428_Pro-Q Emerald 300 Glycoprotein stain



20160429_Sypro Ruby Protein stain (stains all proteins)

1. CandyCane std, 0.25µg of each protein

from

Jason

- 2. rPBP2a, 0.25µg
- 3. PBP2a IP 3.4.2016, 10µl
- 4. PBP2a IP 3.18.2016, 10µl
- 5. IP untreated #2, 10µl
- 6. IP + treated #1, 10µl
- 7. IP 3.22.2016, 10µl
- 8. IP + MIX 3.22.2016, 10µl
- BioRad Precision plus std, 5µl
- 10. STA2; 25.11.2015, 10µl (Herdis)







Supplemental Figure S3.1 **KIKIVPLILIVVVVGFGIYFYASK**

Location: aa 2-26 Precursor Charge State: 3 Theoretical Monoisotopic: 893.8920 *m*/*z* Mass Error: 3.2 ppm



Supplemental Figure S3.2 **DKEINNTIDAIEDK**

Location: aa 27-40 Precursor Charge State: 2 Theoretical Monoisotopic: 809.4019 *m*/*z* Mass Error: 4.1 ppm



Supplemental Figure S3.3 IDAIEDK (Proteinase K)

Location: aa 34-40 Precursor Charge State: 2 Theoretical Monoisotopic: 402.2109 *m*/*z* Mass Error: 0 ppm



Supplemental Figure S3.4 IDAIEDKNFKQ (Proteinase K)

Location: aa 34-44 Precursor Charge State: 3 Theoretical Monoisotopic: 440.8980 *m*/*z* Mass Error: 1.1 ppm



Supplemental Figure S3.5 **DSSYISK**

Location: aa 48-54 Precursor Charge State: 2 Theoretical Monoisotopic: 400.1953 *m*/*z* Mass Error: 1.7 ppm



Supplemental Figure S3.6 **SDNGEVEMTERPIK**

Location: aa 55-68 Precursor Charge State: 2 Theoretical Monoisotopic: 802.8829 *m*/*z* Mass Error: 3.5 ppm



Supplemental Figure S3.7 IYNSLGVK

Location: aa 69-76 Precursor Charge State: 2 Theoretical Monoisotopic: 447.2582 *m*/*z* Mass Error: 0.9 ppm



Supplemental Figure S3.8 **DINIQDR**

Location: aa 77-83 Precursor Charge State: 2 Theoretical Monoisotopic: 437.2249 *m*/*z* Mass Error: 1.8 ppm



Supplemental Figure S3.9 **RVDAQYK**

Location: aa 94-100 Precursor Charge State: 2 Theoretical Monoisotopic: 440.2378 *m*/*z* Mass Error: 1.1 ppm



Supplemental Figure S3.10 **IKTNYGNIDR**

Location: aa 101-110 Precursor Charge State: 3 Theoretical Monoisotopic: 398.5473 *m*/*z* Mass Error: 1.8 ppm



Supplemental Figure S3.11 **TNYGNIDR**

Location: aa 103-110 Precursor Charge State: 2 Theoretical Monoisotopic: 476.7278 *m*/*z* Mass Error: 1.8 ppm



Location: aa 111-118 Precursor Charge State: 2 Theoretical Monoisotopic: 498.2691 *m*/*z* Mass Error: 4.0 ppm



Supplemental Figure S3.13 **LDWDHSVIIPGMQK**

Location: aa 125-138 Precursor Charge State: 3 Theoretical Monoisotopic: 546.9485 *m*/*z* Mass Error: 4.6 ppm



Supplemental Figure S3.14 **DQSIHIENLK**

Location: aa 139-148 Precursor Charge State: 3 Theoretical Monoisotopic: 399.5472 *m*/*z* Mass Error: 3.5 ppm



KMDEYLSDFAK

Location: aa 219-229 Precursor Charge State: 3 Theoretical Monoisotopic: 449.5481 *m*/*z* Mass Error: 0.2 ppm



Supplemental Figure S3.16 **KFHLTTNETESR**

Location: aa 230-241 Precursor Charge State: 3 Theoretical Monoisotopic: 488.2477 *m*/*z* Mass Error: -0.2 ppm



Supplemental Figure S3.17 FHLTTNETESR

Location: aa 231-241 Precursor Charge State: 3 Theoretical Monoisotopic: 445.5494 *m*/*z* Mass Error: 2.2 ppm



Supplemental Figure S3.18 ATSHLLGYVGPINSEELK

Location: aa 248-265 Precursor Charge State: 3 Theoretical Monoisotopic: 643.3423 *m*/*z* Mass Error: 1.6 ppm



Supplemental Figure S3.19 **GYKDDAVIGK**

Location: aa 271-280 Precursor Charge State: 2 Theoretical Monoisotopic: 533.2824 *m*/*z* Mass Error: 3.4 ppm



Supplemental Figure S3.20 **KLQHEDGYR**

Location: aa 290-298 Precursor Charge State: 3 Theoretical Monoisotopic: 382.5281 *m*/*z* Mass Error: -0.3 ppm



Supplemental Figure S3.21 HEDGYRVT (Proteinase K)

Location: aa 293-300 Precursor Charge State: 2 Theoretical Monoisotopic: 488.7278 *m*/*z* Mass Error: 0.6 ppm



Supplemental Figure S3.22 VTIVDDNSNTIAHTLIEK

Location: aa 299-316 Precursor Charge State: 3 Theoretical Monoisotopic: 661.6846 *m*/*z* Mass Error: 2.1 ppm



Supplemental Figure S3.23 IVDDNSNTIAH (Proteinase K)

Location: aa 301-311 Precursor Charge State: 2 Theoretical Monoisotopic: 599.7886 *m*/*z* Mass Error: 0.3 ppm



Supplemental Figure S3.24 **DGKDIQLTIDAK**

Location: aa 320-331 Precursor Charge State: 3 Theoretical Monoisotopic: 439.5734 *m*/*z* Mass Error: 1.1 ppm



Supplemental Figure S3.25 **DIQLTIDAK**

Location: aa 323-331 Precursor Charge State: 2 Theoretical Monoisotopic: 508.7848 *m*/*z* Mass Error: 0.6 ppm



Supplemental Figure S3.26 NDYGSGTAIHPQTGELLALVSTPSYDVYPFMYGMSNEEYNK

Location: aa 342-382 Precursor Charge State: 3 Theoretical Monoisotopic: 1521.3613 *m*/*z* Mass Error: 3.5 ppm



Supplemental Figure S3.27 SNEEYNKL (Proteinase K)

Location: aa 376-383 Precursor Charge State: 2 Theoretical Monoisotopic: 498.7353 *m*/*z* Mass Error: 1.6 ppm



Location: aa 383-394 Precursor Charge State: 3 Theoretical Monoisotopic: 476.6083 *m*/*z* Mass Error: 3.2 ppm



FQITTSPGSTQK

Location: aa 395-406 Precursor Charge State: 2 Theoretical Monoisotopic: 647.8355 *m*/*z* Mass Error: 0.9 ppm



ILTAMIGLNNK

Location: aa 407-417 Precursor Charge State: 2 Theoretical Monoisotopic: 594.3445 *m*/*z* Mass Error: 0.3 ppm



Location: aa 407-417 Precursor Charge State: 2 Theoretical Monoisotopic: 602.3419 *m*/*z* Mass Error: 2.2 ppm



Supplemental Figure S3.32 **TLDDKTSYK**

Location: aa 418-426 Precursor Charge State: 3 Theoretical Monoisotopic: 357.5170 *m*/*z* Mass Error: 2.5 ppm



Supplemental Figure S3.33 **DKSWGGYNVTR**

Location: aa 435-445 Precursor Charge State: 3 Theoretical Monoisotopic: 428.2107 *m*/*z* Mass Error: 1.4 ppm



YEVVNGNIDLK

Location: aa 446-456 Precursor Charge State: 2 Theoretical Monoisotopic: 632.3326 *m*/*z* Mass Error: 0.3 ppm



Supplemental Figure S3.35 **QAIESSDNIFFAR**

Location: aa 457-469 Precursor Charge State: 2 Theoretical Monoisotopic: 749.3703 *m*/*z* Mass Error: 2.3 ppm



Supplemental Figure S3.36 **VALELGSK**

Location: aa 470-477 Precursor Charge State: 2 Theoretical Monoisotopic: 408.7449 *m*/*z* Mass Error: 2.2 ppm



Supplemental Figure S3.37 **KLGVGEDIPSDYPFYNAQISNK**

Location: aa 485-506 Precursor Charge State: 3 Theoretical Monoisotopic: 819.0762 *m*/*z* Mass Error: 1.9 ppm



Supplemental Figure S3.38 LGVGEDIPSDYPFYNAQISNK

Location: aa 486-506 Precursor Charge State: 2 Theoretical Monoisotopic: 776.3779 *m*/*z* Mass Error: 2.2 ppm



Supplemental Figure S3.39 NKNLDNEIL (Proteinase K)

Location: aa 505-513 Precursor Charge State: 2 Theoretical Monoisotopic: 536.7853 *m*/*z* Mass Error: 1.1 ppm



Supplemental Figure S3.40 **NLDNEILLADSGYGQGEILINPVQILSIYSALENNGNINAPHLLK**

Location: aa 507-551 Precursor Charge State: 3 Theoretical Monoisotopic: 1620.8521 *m*/*z* Mass Error: 2.8 ppm



Supplemental Figure S3.41 THKEDIYRSY (Proteinase K)

Location: aa 582-589 Precursor Charge State: 3 Theoretical Monoisotopic: 437.8824 *m*/*z* Mass Error: 1.8 ppm



Supplemental Figure S3.42 **THKEDIYR**

Location: aa 582-589 Precursor Charge State: 3 Theoretical Monoisotopic: 354.5173 *m*/*z* Mass Error: 1.4 ppm



Supplemental Figure S3.43 HKEDIYRSY (Proteinase K)

Location: aa 583-591 Precursor Charge State: 3 Theoretical Monoisotopic: 404.1999 *m*/*z* Mass Error: -0.2 ppm



Supplemental Figure S3.44 **SYANLIGK**

Location: aa 590-597 Precursor Charge State: 2 Theoretical Monoisotopic: 433.2425 *m*/*z* Mass Error: 3.9 ppm



Supplemental Figure S3.45 **SGTAELK**

Location: aa 598-604 Precursor Charge State: 2 Theoretical Monoisotopic: 353.1925 *m*/*z* Mass Error: -0.6 ppm



Supplemental Figure S3.46 QIGWFISYDKDNPNmMMAINVK

Location: aa 613-634 Precursor Charge State: 3 Theoretical Monoisotopic: 877.7517 *m*/*z* Mass Error: -0.1ppm



Supplemental Figure S3.47 ISYDKDNPNMM (Proteinase K)

Location: aa 618-628 Precursor Charge State: 2 Theoretical Monoisotopic: 664.2865 *m*/*z* Mass Error: 2.0 ppm



Supplemental Figure S3.48 YDKDNPNMM (Proteinase K)

Location: aa 620-628 Precursor Charge State: 2 Theoretical Monoisotopic: 564.2284 *m*/*z* Mass Error: 2.0 ppm



Supplemental Figure S3.49 DKDNPNMM (Proteinase K)

Location: aa 621-628 Precursor Charge State: 2 Theoretical Monoisotopic: 482.6968 *m*/*z* Mass Error: 0.8 ppm



Supplemental Figure S3.50 **GMASYNAK**

Location: aa 640-647 Precursor Charge State: 2 Theoretical Monoisotopic: 421.1973 *m*/*z* Mass Error: -0.7 ppm



Supplemental Figure S3.51 **VYDELYENGNK**

Location: aa 652-662 Precursor Charge State: 2 Theoretical Monoisotopic: 672.3093 *m*/*z* Mass Error: 1.8 ppm



Supplemental Figure S3.52 **KYDIDE**

Location: aa 663-668 Precursor Charge State: 2 Theoretical Monoisotopic: 391.6820 *m*/*z* Mass Error: -0.5 ppm



Representative illustration of cyclic peptide rearrangement of source-induced PBP2a_{mecA} N-terminal peptide for precursor m/z = 653.4382.



Representative elution profile for PBP2a_{mecA} as indicated by the extracted ion chromatogram for the *m*/*z* 982.6482 transition ion (fMKKIKIV_L⁺) for both source-induced peptide-like targets. This analysis was performed following PBP2a_{mecA} enrichment and separation performed on the ProSwift RP-4H at 200 µL/min.



Representative illustration of cyclic peptide rearrangement of source-induced PBP2a_{mecC} N-terminal peptide for precursor m/z = 715.4462.



Cross sectional display of reverse phase monolith SPE tip.



Representative elution profile for PBP2a_{mecA} on the monolith solid phase extraction tip as illustrated by extracted ion chromatogram for the *m*/*z* 982.6482 transition ion (fMKKIKIV_L⁺) for both source-induced peptide-like targets. Acetonitrile gradient is indicated by the blue line. Protein separation was performed at 3 µL/min.

