

# Supplementary Materials: Purification and Characterization of Novel Anti-MRSA Peptides Produced by *Brevibacillus* sp. SPR-20

Nuttapon Songnaka <sup>1</sup>, Monthon Lertcanawanichakul <sup>2</sup>, Albert M. Hutapea <sup>3</sup>,

Sucheewin Krobthong <sup>4</sup>, Yodying Yingchutrakul <sup>5</sup>, Apichart Atipairin <sup>1, 6, \*</sup>

**Table S1.** The b-ion and y-ion tables of each anti-MRSA peptide from *Brevibacillus* sp. SPR-20 after peptide fragmentation and mass determination by tandem mass spectrometry. (A) P1, (B) P2, (C) P3, (D) P4, and (E) P5.

## A. Peptide P1

| #  | b       | b-H2O   | b-NH3   | a       | c       | b (2+) | Seq | y       | y-H2O   | y-NH3   | z       | z'      | y (2+) | #  |
|----|---------|---------|---------|---------|---------|--------|-----|---------|---------|---------|---------|---------|--------|----|
| 1  | 100.08  | 82.07   | 83.05   | 72.08   | 117.10  | 50.54  | V   |         |         |         |         |         |        | 15 |
| 2  | 199.18  | 181.09  | 182.12  | 171.15  | 216.17  | 100.07 | V   | 1471.96 | 1453.95 | 1454.93 | 1454.93 | 1455.94 | 736.48 | 14 |
| 3  | 298.21  | 280.16  | 281.19  | 270.22  | 315.24  | 149.61 | V   | 1372.93 | 1354.93 | 1355.93 | 1355.93 | 1356.87 | 686.95 | 13 |
| 4  | 412.32  | 394.25  | 395.23  | 384.26  | 429.28  | 206.63 | N   | 1273.87 | 1255.87 | 1256.87 | 1256.87 | 1257.85 | 637.41 | 12 |
| 5  | 511.38  | 493.31  | 494.30  | 483.33  | 528.35  | 256.16 | V   | 1159.79 | 1141.79 | 1142.78 | 1142.78 | 1143.80 | 580.39 | 11 |
| 6  | 624.41  | 606.40  | 607.38  | 596.41  | 641.44  | 312.22 | L   | 1060.73 | 1042.71 | 1043.72 | 1043.72 | 1044.69 | 530.86 | 10 |
| 7  | 723.48  | 705.47  | 706.45  | 695.48  | 740.50  | 362.24 | V   | 947.65  | 929.63  | 930.64  | 930.64  | 931.62  | 474.31 | 9  |
| 8  | 851.56  | 833.56  | 834.54  | 823.58  | 868.60  | 426.30 | K   | 848.58  | 830.57  | 831.56  | 831.56  | 832.54  | 425.30 | 8  |
| 9  | 950.63  | 932.61  | 933.61  | 922.65  | 967.67  | 475.82 | V   | 720.49  | 702.48  | 703.44  | 703.44  | 704.45  | 360.73 | 7  |
| 10 | 1063.71 | 1045.69 | 1046.71 | 1035.72 | 1080.75 | 532.30 | L   | 621.42  | 603.41  | 604.37  | 604.37  | 605.38  | 311.20 | 6  |
| 11 | 1160.80 | 1142.78 | 1143.80 | 1132.78 | 1177.80 | 580.89 | P   | 508.34  | 490.33  | 491.29  | 491.29  | 492.31  | 254.66 | 5  |
| 12 | 1257.85 | 1239.82 | 1240.80 | 1229.83 | 1274.86 | 629.41 | P   | 411.25  | 393.24  | 394.23  | 394.23  | 395.24  | 206.13 | 4  |
| 13 | 1354.93 | 1336.85 | 1337.86 | 1326.89 | 1371.91 | 677.94 | P   | 314.22  | 296.19  | 297.17  | 297.17  | 298.21  | 157.60 | 3  |
| 14 | 1453.95 | 1435.94 | 1436.92 | 1425.96 | 1470.98 | 727.47 | V   | 217.19  | 199.18  | 200.13  | 200.13  | 201.14  | 109.08 | 2  |
| 15 |         |         |         |         |         |        | V   | 118.12  | 100.08  | 101.06  | 101.06  | 102.07  | 59.54  | 1  |

## B. Peptide P2

| #  | b       | b-H2O   | b-NH3   | a       | c       | b (2+) | Seq | y       | y-H2O   | y-NH3   | z       | z'      | y (2+) | #  |
|----|---------|---------|---------|---------|---------|--------|-----|---------|---------|---------|---------|---------|--------|----|
| 1  | 100.08  | 82.07   | 83.05   | 72.08   | 117.10  | 50.54  | V   |         |         |         |         |         |        | 14 |
| 2  | 199.18  | 181.10  | 182.12  | 171.15  | 216.17  | 100.07 | V   | 1517.95 | 1499.94 | 1500.92 | 1500.92 | 1501.93 | 759.46 | 13 |
| 3  | 330.19  | 312.13  | 313.25  | 302.33  | 347.21  | 165.59 | M   | 1418.93 | 1400.85 | 1401.86 | 1401.86 | 1402.86 | 710.47 | 12 |
| 4  | 444.23  | 426.22  | 427.20  | 416.23  | 461.26  | 222.61 | N   | 1287.89 | 1269.87 | 1270.87 | 1270.87 | 1271.82 | 644.42 | 11 |
| 5  | 557.31  | 539.30  | 540.29  | 529.32  | 574.34  | 279.16 | L   | 1173.81 | 1155.80 | 1156.80 | 1156.80 | 1157.78 | 587.91 | 10 |
| 6  | 670.40  | 652.39  | 653.37  | 642.40  | 687.42  | 335.70 | L   | 1060.73 | 1042.72 | 1043.72 | 1043.72 | 1044.69 | 530.86 | 9  |
| 7  | 769.46  | 751.45  | 752.44  | 741.47  | 786.49  | 385.23 | V   | 947.65  | 929.64  | 930.60  | 930.60  | 931.61  | 474.31 | 8  |
| 8  | 897.56  | 879.55  | 880.53  | 869.56  | 914.59  | 449.28 | K   | 848.58  | 830.57  | 831.57  | 831.57  | 832.54  | 425.21 | 7  |
| 9  | 996.62  | 978.60  | 979.60  | 968.62  | 1013.66 | 498.81 | V   | 720.49  | 702.48  | 703.44  | 703.44  | 704.45  | 360.73 | 6  |
| 10 | 1109.70 | 1091.67 | 1092.69 | 1081.72 | 1126.74 | 555.36 | L   | 621.42  | 603.42  | 604.37  | 604.37  | 605.38  | 311.15 | 5  |
| 11 | 1237.79 | 1219.80 | 1220.78 | 1209.81 | 1254.83 | 619.40 | K   | 508.34  | 490.33  | 491.29  | 491.29  | 492.29  | 254.66 | 4  |
| 12 | 1400.85 | 1382.83 | 1383.84 | 1372.88 | 1417.90 | 700.43 | Y   | 380.25  | 362.24  | 363.19  | 363.19  | 364.20  | 190.61 | 3  |
| 13 | 1499.94 | 1481.93 | 1482.91 | 1471.94 | 1516.97 | 750.47 | V   | 217.19  | 199.18  | 200.13  | 200.13  | 201.10  | 109.08 | 2  |
| 14 |         |         |         |         |         |        | V   | 118.09  | 100.08  | 101.06  | 101.06  | 102.07  | 59.54  | 1  |

