

Identified Spike Peptides

| Year | Weight | Sequence* | Protein identification probability (%) | ECRIST Score | ECRIST AminoAc | Modifications | Observed Mass (Da) | Actual Mass (Da) | Charge | Delta C | Delta MS | Retention Time | # Other Peptides | Other Peptides | Total Ion Chromatogram (PIC) | Spectrum ID | Protein Name | Protein Score |
|------|--------|-----------|--|--------------|----------------|---------------|--------------------|------------------|--------|---------|----------|----------------|------------------|----------------|------------------------------|-------------|--------------|---------------|
| 2014 | 0.0001 | AKKPK | 0.0001 | 4.82 | 4.82 | | 1453.07 | 1453.07 | 2 | 0.00 | 1.00 | 12.18 | 1 | AKKPK | 541.10 | Spectrum ID | Protein Name | Protein Score |
| 2014 | 0.0001 | AKKPK | 0.0001 | 4.82 | 4.82 | | 1453.07 | 1453.07 | 2 | 0.00 | 1.00 | 12.18 | 1 | AKKPK | 541.10 | Spectrum ID | Protein Name | Protein Score |
| 2014 | 0.0001 | AKKPK | 0.0001 | 4.82 | 4.82 | | 1453.07 | 1453.07 | 2 | 0.00 | 1.00 | 12.18 | 1 | AKKPK | 541.10 | Spectrum ID | Protein Name | Protein Score |
| 2014 | 0.0001 | AKKPK | 0.0001 | 4.82 | 4.82 | | 1453.07 | 1453.07 | 2 | 0.00 | 1.00 | 12.18 | 1 | AKKPK | 541.10 | Spectrum ID | Protein Name | Protein Score |

* Only the first modification is listed here. The ECRIST score was calculated following the sequence number of the original type sequence. The sequence number is also modified to indicate the charge and MS tag in the case of in-house tags, to insert an asterisk (*) designates the ECRIST score.

* Legend for modifications: acetylation (Ac), carbamidomethyl (CM), phosphorylation (Ph), palmitoylation (Pal), oxidation (O), n-butylamine (NB), and hydroxylation (H).

Identified M proteins

| Bio Sample Category / Sequence Coverage ^a | Protein | Accession | Category/Bio Sample | Protein identification probability (Prob) | Exclusive unique peptide count (#Pep) | Exclusive unique spectrum count (#Unique) | Total spectrum count (#Spec) | Percentage of total spectra (%Spec) | Percentage of amino acids identified (%Cov) | Protein molecular mass (kDa) |
|---|--|------------|---|---|---------------------------------------|---|------------------------------|-------------------------------------|---|------------------------------|
| 1_Control_Purified_Virions | | | | | | | | | | |
| ADAM17H24 (96%) 25,1215 Da Membrane glycoprotein OS=Severe acute respiratory syndrome coronavirus 2 OX=2697049 GN=M PE=4 SV=1 0 exclusive unique peptides, 0 exclusive unique spectra, 1 total spectra, 21,222 amino acids (10% coverage) | Membrane glycoprotein OS=Severe acute respiratory syndrome coronavirus 2 OX=2697049 GN=M PE=4 SV=1 | ADA7M1H24 | 1_Control_Purified_virions_1 | 64% | 0 | 0 | 1 | 0.0021% | 9.9% | 25 kDa |
| ADAM17 (96%) 25,1492 Da Membrane protein OS=Severe acute respiratory syndrome coronavirus 2 OX=2697049 GN=M PE=3 SV=1 0 exclusive unique peptides, 0 exclusive unique spectra, 1 total spectra, 21,222 amino acids (10% coverage) | Membrane protein OS=Severe acute respiratory syndrome coronavirus 2 OX=2697049 GN=M PE=3 SV=1 | AD6MM4NE17 | 1_Control_Purified_virions_1 | 40% | 0 | 0 | 1 | 0.0021% | 9.9% | 25 kDa |
| 2_Mock_Treated_Purified_Virions | | | | | | | | | | |
| ADAM17H24 (71%) 25,1215 Da Membrane glycoprotein OS=Severe acute respiratory syndrome coronavirus 2 OX=2697049 GN=M PE=4 SV=1 0 exclusive unique peptides, 0 exclusive unique spectra, 3 total spectra, 381,222 amino acids (17% coverage) | Membrane glycoprotein OS=Severe acute respiratory syndrome coronavirus 2 OX=2697049 GN=M PE=4 SV=1 | ADA7M1H24 | 2_Mock_Purified_Virions_mock_treated_1 | 71% | 0 | 0 | 3 | 0.0063% | 17.1% | 25 kDa |
| ADAM17 (66%) 25,1492 Da Membrane protein OS=Severe acute respiratory syndrome coronavirus 2 OX=2697049 GN=M PE=3 SV=1 0 exclusive unique peptides, 0 exclusive unique spectra, 3 total spectra, 381,222 amino acids (17% coverage) | Membrane protein OS=Severe acute respiratory syndrome coronavirus 2 OX=2697049 GN=M PE=3 SV=1 | AD6MM4NE17 | 2_Mock_Purified_Virions_mock_treated_1 | 46% | 0 | 0 | 3 | 0.0063% | 17.1% | 25 kDa |
| 3_PNGase-F_Treated_Purified_Virions | | | | | | | | | | |
| ADAM17H24 (96%) 25,1215 Da Membrane glycoprotein OS=Severe acute respiratory syndrome coronavirus 2 OX=2697049 GN=M PE=4 SV=1 0 exclusive unique peptides, 0 exclusive unique spectra, 15 total spectra, 312,222 amino acids (24% coverage) | Membrane glycoprotein OS=Severe acute respiratory syndrome coronavirus 2 OX=2697049 GN=M PE=4 SV=1 | ADA7M1H24 | 3_PNG+purified_virions_PNGase-F_treated_1 | 96% | 0 | 0 | 15 | 0.0314% | 23.9% | 25 kDa |
| ADAM17 (97%) 25,1492 Da Membrane protein OS=Severe acute respiratory syndrome coronavirus 2 OX=2697049 GN=M PE=3 SV=1 0 exclusive unique peptides, 0 exclusive unique spectra, 15 total spectra, 312,222 amino acids (24% coverage) | Membrane protein OS=Severe acute respiratory syndrome coronavirus 2 OX=2697049 GN=M PE=3 SV=1 | AD6MM4NE17 | 3_PNG+purified_virions_PNGase-F_treated_1 | 97% | 0 | 0 | 15 | 0.0314% | 23.9% | 25 kDa |
| 4_Inactivated_PNGase-F_Treated_Purified_Virions | | | | | | | | | | |
| ADAM17H24 (92%) 25,1215 Da Membrane glycoprotein OS=Severe acute respiratory syndrome coronavirus 2 OX=2697049 GN=M PE=4 SV=1 0 exclusive unique peptides, 0 exclusive unique spectra, 13 total spectra, 40,222 amino acids (20% coverage) | Membrane glycoprotein OS=Severe acute respiratory syndrome coronavirus 2 OX=2697049 GN=M PE=4 SV=1 | ADA7M1H24 | 4_Inactiv+purified_virions_PNGase-F_inactivated_1 | 92% | 0 | 0 | 13 | 0.0303% | 20.3% | 25 kDa |
| ADAM17 (77%) 25,1492 Da Membrane protein OS=Severe acute respiratory syndrome coronavirus 2 OX=2697049 GN=M PE=3 SV=1 0 exclusive unique peptides, 0 exclusive unique spectra, 13 total spectra, 40,222 amino acids (20% coverage) | Membrane protein OS=Severe acute respiratory syndrome coronavirus 2 OX=2697049 GN=M PE=3 SV=1 | AD6MM4NE17 | 4_Inactiv+purified_virions_PNGase-F_inactivated_1 | 37% | 0 | 0 | 13 | 0.0303% | 20.3% | 25 kDa |

^a The identified peptides are highlighted in orange; modified Cys residues are highlighted in green.

^b NDM: Asn to Asp modification. The NDM annotation was manually added following the accession number of the original Spike sequence to indicate that the asparagine (N) residues were in-silico modified to aspartic acid (D) by an in-house script, to account for an experimental N-deglycosylation by PNGase-F treatment.

