

# Comprehensive profiling of the native and modified peptidomes of raw bovine milk and processed milk products

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**Table S1:** List of targeted dynamic modifications corresponding to Amadori products (red), advanced glycation end-products (green), and oxidation/carbonylation (blue).

| Modification   | Mass shift [Da] | Amino acid residue  |
|--|-----------------|---------------------|
| Acetylation <sup>c</sup>                             | +42.011         | K                   |
| Acrolein <sup>c</sup>                                | +56.026         | C, H, K             |
| Argpyrimidine <sup>e</sup>                           | +80.026         | R                   |
| Carboxyethyl <sup>f</sup>                            | +72.021         | K, R                |
| Carboxymethyl <sup>a</sup>                           | +58.005         | K, R                |
| Crotonaldehyde <sup>c</sup>                          | +70.042         | C, H, K             |
| Formylation <sup>a</sup>                             | +27.995         | K                   |
| Glutamic semialdehyde <sup>b</sup>                   | -43.053         | R                   |
| Glyceraldehyde-derived pyridinium <sup>f</sup>       | +109.029        | K                   |
| Glycerinyl lysine <sup>c</sup>                       | +88.016         | K                   |
| Glyoxal-derived hydroimidazolium <sup>e</sup>        | +39.995         | R                   |
| Hexosylation <sup>a</sup> (Hex)                      | +162.053        | K                   |
| Lactosylation <sup>a</sup> (Lac)                     | +324.106        | K                   |
| Methylglyoxal-derived hydroimidazolones <sup>e</sup> | +54.011         | R                   |
| Oxalic acid monolysinylamide <sup>f</sup>            | +71.985         | K                   |
| Oxidation <sup>b</sup> (Ox)                          | +15.995         | P, C, W, Y          |
| Pentenal <sup>c</sup>                                | +84.060         | C, H, K             |
| Pyrraline <sup>f</sup>                               | +108.021        | K                   |
| Tetrahydropyrimidine <sup>e</sup>                    | +144.042        | R                   |
| +14 Da Carbonylation <sup>b</sup>                    | +13.979         | A, E, I, L, K, Q, V |
| 2-Amino-3-ketobutyric acid <sup>b</sup> (T(Ox))      | -2.016          | T                   |
| 2-Aminoadipic semialdehyde <sup>b</sup>              | -1.032          | K                   |
| 4-Hydroxy-2-hexanal <sup>d</sup>                     | +114.068        | C, H, K             |
| 4-Hydroxy-2-nonenal <sup>d</sup>                     | +156.115        | C, H, K             |
| 4-Oxo-2-hexanal <sup>d</sup>                         | +112.052        | C, H, K             |
| 4-Oxo-2-nonenal <sup>d</sup>                         | +154.099        | C, H, K             |

<sup>a-f</sup> denote the templates in which modifications were searched together within Proteome Discoverer. Each template additionally contained oxidation of methionine and phosphorylation of serine as dynamic modifications. As PEAKS allows targeting many PTMs, all modifications were included as dynamic modifications.

**Table S2:** Unmodified peptides identified by both Proteome Discoverer 2.2 (Xcorr) and PEAKS Studio 10.5 (-10lgP) sorted by proteins (if present signal peptides were removed). An “x” indicates that the peptides was present in RM, UHT milk or IF, whereas a “blank” indicates that it was not detected. Methionine oxidation (M(Ox)) and phosphorylation of serine\* (S(Phospho)) were considered as variable modifications.

| Nr.                             | Start pos. | End pos. | Sequence             | Modification | z       | m/z     | t <sub>r</sub> (min) | Xcorr | -10lgP | RM <sup>a</sup> | UH T <sup>a</sup> | IF <sup>a</sup> | Literature (milk <sup>1-6</sup> , colostrum <sup>7</sup> ) |
|---------------------------------|------------|----------|----------------------|--------------|---------|---------|----------------------|-------|--------|-----------------|-------------------|-----------------|--|
| <b>Alpha-S1-casein (P02662)</b> |            |          |                      |              |         |         |                      |       |        |                 |                   |                 |  |
| 1                               | 1          | 21       | RPKHPHQGLPQEVLNENLL  | none         | 3 (4)   | 820.799 | 38.94                | 3.8   | 57.7   | x               | x                 | x               | 1; 3; 5  |
| 2                               | 1          | 22       | RPKHPHQGLPQEVLNENLLR | none         | 4 (5)   | 654.878 | 35.38                | 3.5   | 44.8   | x               | x                 | x               | 1; 3; 5  |
| 3                               | 4          | 19       | HPIKHQGLPQEVLNEN     | none         | 3       | 618.325 | 27.28                | 3.3   | 36.2   | x               | x                 | x               | 1; 7; 5  |
| 4                               | 4          | 21       | HPIKHQGLPQEVLNENLL   | none         | 3 (2,4) | 693.717 | 43.32                | 3.4   | 68.6   | x               | x                 | x               | 1; 3; 5  |
| 5                               | 4          | 22       | HPIKHQGLPQEVLNENLLR  | none         | 3 (4)   | 745.749 | 39.00                | 5.0   | 59.4   | x               | x                 | x               | 1; 3; 5  |
| 6                               | 4          | 23       | HPIKHQGLPQEVLNENLLRF | none         | 3       | 794.773 | 48.95                | 5.0   | 54.4   | x               | x                 |                 | 5  |
| 7                               | 7          | 16       | KHQGLPQEVL           | none         | 2       | 574.824 | 29.04                | 2.5   | 56.9   | x               | x                 | x               |  |
| 8                               | 7          | 23       | KHQGLPQEVLNENLLRF    | none         | 3       | 679.041 | 51.10                | 3.3   | 58.3   |                 |                   | x               |  |
| 9                               | 8          | 21       | HQGLPQEVLNENLL       | none         | 2       | 802.425 | 49.46                | 2.9   | 58.9   | x               | x                 | x               | 1; 5   |
| 10                              | 8          | 22       | HQGLPQEVLNENLLR      | none         | 3 (2)   | 587.320 | 44.19                | 4.7   | 92.6   | x               | x                 | x               | 1; 3; 5  |
| 11                              | 9          | 17       | QGLPQEVLN            | none         | 2       | 499.269 | 35.17                | 1.7   | 43.1   |                 |                   | x               |  |
| 12                              | 9          | 21       | QGLPQEVLNENLL        | none         | 2       | 733.897 | 55.28                | 3.4   | 53.5   |                 |                   | x               | 5  |
| 13                              | 9          | 22       | QGLPQEVLNENLLR       | none         | 2       | 811.948 | 49.07                | 3.4   | 74.6   | x               | x                 | x               | 5  |
| 14                              | 9          | 23       | QGLPQEVLNENLLRF      | none         | 2       | 885.482 | 59.94                | 3.3   | 77.2   |                 |                   | x               |  |
| 15                              | 10         | 17       | GLPQEVLN             | none         | 2       | 435.239 | 34.78                | 1.9   | 46.4   | x               | x                 | x               | 1  |
| 16                              | 10         | 18       | GLPQEVLNE            | none         | 2       | 499.761 | 38.33                | 2.2   | 46.7   |                 |                   | x               |  |
| 17                              | 10         | 20       | GLPQEVLNENL          | none         | 2       | 613.325 | 47.92                | 2.0   | 38.0   | x               | x                 | x               | 5; 7   |
| 18                              | 10         | 21       | GLPQEVLNENLL         | none         | 2       | 669.867 | 55.75                | 2.8   | 45.7   | x               | x                 | x               | 1; 3; 5  |
| 19                              | 10         | 22       | GLPQEVLNENLLR        | none         | 2       | 747.917 | 49.28                | 4.3   | 74.3   | x               | x                 | x               | 1; 3; 5; 7   |
| 20                              | 10         | 23       | GLPQEVLNENLLRF       | none         | 2       | 821.451 | 60.49                | 4.0   | 75.2   | x               | x                 | x               | 1; 5   |
| 21                              | 10         | 24       | GLPQEVLNENLLRFF      | none         | 2       | 894.988 | 70.69                | 3.9   | 55.5   |                 |                   | x               |  |
| 22                              | 11         | 20       | LPQEVLNENL           | none         | 2       | 584.813 | 42.74                | 2.6   | 50.3   | x               | x                 |                 | 1  |
| 23                              | 11         | 21       | LPQEVLNENLL          | none         | 2       | 641.357 | 51.48                | 2.2   | 42.9   | x               | x                 | x               | 1; 3; 5  |
| 24                              | 11         | 22       | LPQEVLNENLLR         | none         | 2       | 719.407 | 44.47                | 3.8   | 68.1   | x               | x                 | x               |  |

| Nr. | Start pos. | End pos. | Sequence             | Modification | z     | m/z      | t <sub>r</sub> (min) | Xcorr | -10lgP | RM <sup>a</sup> | UH T <sup>a</sup> | IF <sup>a</sup> | Literature (milk <sup>1-6</sup> , colostrum <sup>7</sup> ) |
|-----|------------|----------|----------------------|--------------|-------|----------|----------------------|-------|--------|-----------------|-------------------|-----------------|--|
| 25  | 11         | 23       | LPQEVLNENLLRF        | none         | 2 (3) | 792.941  | 56.68                | 3.7   | 70.7   | x               | x                 | x               | 1; 3; 5; 7   |
| 26  | 13         | 22       | QEVLNENLLR           | none         | 2     | 614.337  | 37.50                | 2.6   | 48.7   | x               | x                 | x               | 1; 3; 5  |
| 27  | 13         | 23       | QEVLNENLLRF          | none         | 2     | 687.873  | 51.93                | 2.7   | 56.3   |                 | x                 |                 | 5  |
| 28  | 14         | 21       | EVLNENLL             | none         | 2     | 472.258  | 44.55                | 2.2   | 39.6   |                 | x                 |                 | 1  |
| 29  | 14         | 22       | EVLNENLLR            | none         | 2     | 550.309  | 36.43                | 2.4   | 50.8   | x               | x                 | x               | 1; 4   |
| 30  | 14         | 23       | EVLNENLLRF           | none         | 2     | 623.844  | 51.49                | 2.7   | 53.6   | x               | x                 | x               | 1; 5; 7  |
| 31  | 14         | 24       | EVLNENLLRFF          | none         | 2     | 697.379  | 63.20                | 2.8   | 43.5   |                 | x                 |                 |  |
| 32  | 15         | 22       | VLNENLLR             | none         | 2     | 485.786  | 32.27                | 3.1   | 50.2   | x               | x                 | x               | 1  |
| 33  | 15         | 23       | VLNENLLRF            | none         | 2     | 559.321  | 48.86                | 2.8   | 55.9   | x               | x                 | x               | 1; 5   |
| 34  | 16         | 22       | LLENLLR              | none         | 2     | 436.252  | 28.15                | 2.6   | 38.8   | x               | x                 |                 | 1  |
| 35  | 16         | 23       | LLENLLRF             | none         | 2     | 509.787  | 46.08                | 3.2   | 49.0   | x               | x                 | x               | 1; 5   |
| 36  | 16         | 24       | LLENLLRFF            | none         | 2     | 583.321  | 58.93                | 2.9   | 51.5   | x               | x                 | x               | 5  |
| 37  | 17         | 23       | NENLLRF              | none         | 2     | 453.244  | 40.95                | 2.4   | 39.8   | x               | x                 | x               | 1; 4   |
| 38  | 17         | 24       | NENLLRFF             | none         | 2     | 526.779  | 55.49                | 2.9   | 46.7   | x               | x                 | x               | 1; 5   |
| 39  | 23         | 33       | FFVAPFPEVFG          | none         | 2     | 628.821  | 70.01                | 1.9   | 57.0   | x               | x                 |                 | 1; 5   |
| 40  | 23         | 34       | FFVAPFPEVFGK         | none         | 2     | 692.869  | 60.89                | 2.8   | 67.1   | x               | x                 | x               | 1; 3; 5  |
| 41  | 23         | 35       | FFVAPFPEVFGKE        | none         | 2     | 757.390  | 61.19                | 3.4   | 76.5   | x               | x                 |                 | 5  |
| 42  | 23         | 36       | FFVAPFPEVFGKEK       | none         | 2 (3) | 821.437  | 55.07                | 3.1   | 73.0   | x               | x                 | x               | 1; 3; 5  |
| 43  | 23         | 37       | FFVAPFPEVFGKEKV      | none         | 2 (3) | 870.972  | 57.29                | 3.3   | 75.3   | x               | x                 | x               | 5  |
| 44  | 23         | 39       | FFVAPFPEVFGKEKVNE    | none         | 2 (3) | 992.515  | 55.58                | 3.9   | 85.0   | x               | x                 | x               | 1; 3; 5  |
| 45  | 23         | 41       | FFVAPFPEVFGKEKVNELS  | none         | 2 (3) | 1092.573 | 58.00                | 3.2   | 84.2   | x               | x                 | x               | 5  |
| 46  | 23         | 42       | FFVAPFPEVFGKEKVNELSK | none         | 4 (3) | 578.813  | 53.57                | 1.8   | 40.2   | x               | x                 | x               | 5  |
| 47  | 24         | 32       | FVAPFPEVF            | none         | 2     | 526.775  | 63.22                | 2.4   | 51.6   | x               | x                 | x               | 1; 3; 5  |
| 48  | 24         | 33       | FVAPFPEVFG           | none         | 2     | 555.286  | 62.41                | 2.6   | 68.8   | x               | x                 | x               | 1; 5   |
| 49  | 24         | 34       | FVAPFPEVFGK          | none         | 2     | 619.334  | 53.66                | 2.5   | 56.7   | x               | x                 | x               | 1; 3; 5; 7   |
| 50  | 24         | 35       | FVAPFPEVFGKE         | none         | 2     | 683.854  | 54.21                | 2.7   | 72.1   | x               | x                 | x               | 5  |
| 51  | 24         | 36       | FVAPFPEVFGKEK        | none         | 2 (3) | 747.903  | 48.16                | 3.0   | 76.5   | x               | x                 | x               | 1; 5   |
| 52  | 24         | 37       | FVAPFPEVFGKEKV       | none         | 2 (3) | 797.437  | 51.04                | 3.5   | 73.2   | x               | x                 | x               | 1; 2; 5; 7   |
| 53  | 24         | 41       | FVAPFPEVFGKEKVNELS   | none         | 2 (3) | 1019.038 | 52.38                | 3.3   | 73.9   | x               | x                 | x               |  |

| Nr. | Start pos. | End pos. | Sequence                | Modification | z     | m/z     | t <sub>r</sub> (min) | Xcorr | -10lgP | RM <sup>a</sup> | UH T <sup>a</sup> | IF <sup>a</sup> | Literature (milk <sup>1-6</sup> , colostrum <sup>7</sup> ) |
|-----|------------|----------|-------------------------|--------------|-------|---------|----------------------|-------|--------|-----------------|-------------------|-----------------|--|
| 54  | 25         | 32       | VAPFPEVF                | none         | 2     | 453.241 | 55.28                | 1.8   | 46.5   | x               | x                 | x               | 1; 5   |
| 55  | 25         | 33       | VAPFPEVFG               | none         | 2     | 481.751 | 54.34                | 2.5   | 61.2   | x               | x                 | x               | 1; 5   |
| 56  | 25         | 34       | VAPFPEVFGK              | none         | 2     | 545.799 | 45.43                | 1.4   | 50.7   | x               | x                 | x               | 1; 5   |
| 57  | 25         | 35       | VAPFPEVFGKE             | none         | 2     | 610.322 | 46.21                | 2.1   | 58.8   | x               | x                 | x               | 1; 5; 7  |
| 58  | 25         | 36       | VAPFPEVFGKEK            | none         | 2     | 674.368 | 39.75                | 2.0   | 72.9   | x               | x                 | x               | 2; 5   |
| 59  | 25         | 37       | VAPFPEVFGKEKV           | none         | 2 (3) | 723.903 | 43.89                | 2.9   | 73.1   | x               | x                 | x               | 1; 2; 5  |
| 60  | 25         | 41       | VAPFPEVFGKEKVNELS       | none         | 2     | 945.505 | 46.15                | 2.5   | 70.8   | x               | x                 | x               |  |
| 61  | 26         | 33       | APFPEVFG                | none         | 2     | 432.218 | 51.00                | 1.5   | 40.1   | x               | x                 |                 | 1; 3; 5  |
| 62  | 26         | 34       | APFPEVFGK               | none         | 2     | 496.265 | 42.16                | 2.7   | 66.3   | x               | x                 | x               | 1  |
| 63  | 26         | 35       | APFPEVFGKE              | none         | 2     | 560.786 | 42.90                | 3.2   | 77.3   | x               | x                 | x               | 1; 3; 5  |
| 64  | 26         | 36       | APFPEVFGKEK             | none         | 2 (3) | 624.835 | 36.41                | 2.8   | 71.3   | x               | x                 | x               | 1; 3; 5  |
| 65  | 26         | 37       | APFPEVFGKEKV            | none         | 2 (3) | 674.368 | 40.86                | 3.5   | 82.8   | x               | x                 | x               | 1; 5   |
| 66  | 26         | 39       | APFPEVFGKEKVNE          | none         | 3 (2) | 530.944 | 38.68                | 3.0   | 68.8   | x               | x                 | x               | 1; 5   |
| 67  | 26         | 40       | APFPEVFGKEKVNL          | none         | 3     | 568.637 | 46.12                | 2.7   | 47.5   | x               | x                 | x               |  |
| 68  | 26         | 41       | APFPEVFGKEKVNELS        | none         | 2 (3) | 895.971 | 43.69                | 2.5   | 80.6   | x               | x                 | x               | 1  |
| 69  | 27         | 34       | PFPEVFGK                | none         | 2     | 460.747 | 45.54                | 2.1   | 51.0   | x               | x                 | x               |  |
| 70  | 27         | 36       | PFPEVFGKEK              | none         | 2     | 589.315 | 39.85                | 3.0   | 61.5   | x               | x                 | x               |  |
| 71  | 27         | 37       | PFPEVFGKEKV             | none         | 3 (2) | 426.236 | 47.50                | 2.1   | 40.3   | x               | x                 | x               | 2; 5   |
| 72  | 28         | 34       | FPEVFGK                 | none         | 2     | 412.221 | 36.92                | 2.4   | 55.6   | x               | x                 | x               |  |
| 73  | 28         | 36       | FPEVFGKEK               | none         | 2     | 540.788 | 31.18                | 2.5   | 53.6   | x               | x                 | x               | 1  |
| 74  | 28         | 37       | FPEVFGKEKV              | none         | 2     | 590.323 | 36.71                | 2.9   | 61.2   | x               | x                 | x               | 1; 5   |
| 75  | 35         | 58       | EKNELSKDIGSESTEDQAMEDIK | none         | 3 (4) | 899.092 | 36.84                | 6.8   | 99.4   | x               | x                 | x               |  |
| 76  | 35         | 58       | EKNELSKDIGSESTEDQAmEDIK | M20(Ox)      | 3 (4) | 904.427 | 31.78                | 7.2   | 83.1   | x               | x                 | x               |  |
| 77  | 35         | 58       | EKNELSKDIGSeSTEDQAmEDIK | S14(Phospho) | 3     | 925.750 | 38.67                | 6.2   | 55.2   | x               | x                 | x               | 5  |
| 78  | 37         | 58       | VNELSKDIGSESTEDQAMEDIK  | none         | 3     | 813.379 | 38.03                | 5.6   | 85.0   | x               | x                 | x               | 5  |
| 79  | 37         | 58       | VNELSKDIGSESTEDQAmEDIK  | M18(Ox)      | 3     | 818.711 | 32.25                | 6.0   | 81.1   | x               | x                 | x               |  |
| 80  | 37         | 58       | VNELSKDIGSeSTEDQAMEDIK  | S12(Phospho) | 3     | 840.034 | 40.51                | 6.9   | 69.5   | x               | x                 | x               |  |
| 81  | 38         | 53       | NELSKDIGSESTEDQA        | none         | 2     | 861.887 | 26.89                | 4.6   | 80.3   | x               | x                 | x               | 5  |
| 82  | 43         | 58       | DIGSESTEDQAMEDIK        | none         | 2     | 884.384 | 34.89                | 4.9   | 99.3   | x               | x                 | x               |  |

| Nr. | Start pos. | End pos. | Sequence                  | Modification | z         | m/z      | t <sub>r</sub> (min) | Xcorr | -10lgP | RM <sup>a</sup> | UH T <sup>a</sup> | IF <sup>a</sup> | Literature (milk <sup>1-6</sup> , colostrum <sup>7</sup> ) |
|-----|------------|----------|---------------------------|--------------|-----------|----------|----------------------|-------|--------|-----------------|-------------------|-----------------|--|
| 83  | 43         | 58       | DIGSESTEDQAmEDIK          | M12(Ox)      | 2         | 892.378  | 27.47                | 5.0   | 94.7   | x               | x                 |                 |  |
| 84  | 43         | 58       | DIGSEsTEDQAMEDIK          | S6(Phospho)  | 2         | 924.367  | 38.89                | 4.8   | 74.7   | x               | x                 | x               |  |
| 85  | 44         | 58       | IGSESTEDQAmEDIK           | M11(Ox)      | 2         | 834.865  | 24.02                | 3.4   | 59.9   | x               | x                 |                 |  |
| 86  | 69         | 79       | EEIVPNsVEQK               | S7(Phospho)  | 2         | 676.311  | 26.67                | 2.5   | 39.0   |                 |                   | x               |  |
| 87  | 80         | 90       | HIQKEDVPSER               | none         | 3 (2)     | 669.342  | 13.87                | 4.1   | 54.9   | x               | x                 | x               | 1; 3; 4; 5   |
| 88  | 80         | 91       | HIQKEDVPSERY              | none         | 2 (3)     | 750.875  | 19.18                | 3.1   | 63.8   | x               | x                 | x               | 1; 3; 5  |
| 89  | 80         | 92       | HIQKEDVPSERYL             | none         | 3 (2)     | 538.614  | 27.07                | 3.5   | 74.9   | x               | x                 | x               | 1; 5   |
| 90  | 80         | 93       | HIQKEDVPSERYLG            | none         | 3 (2)     | 557.621  | 25.35                | 4.5   | 61.2   | x               | x                 | x               | 1; 3; 5  |
| 91  | 80         | 94       | HIQKEDVPSERYLGY           | none         | 3         | 611.975  | 30.72                | 4.5   | 76.5   | x               | x                 | x               | 1  |
| 92  | 80         | 95       | HIQKEDVPSERYLGYL          | none         | 3         | 649.672  | 40.11                | 3.6   | 51.9   | x               |                   | x               |  |
| 93  | 80         | 96       | HIQKEDVPSERYLGYLE         | none         | 3         | 692.686  | 38.90                | 3.8   | 54.7   | x               |                   | x               |  |
| 94  | 80         | 97       | HIQKEDVPSERYLGYLEQ        | none         | 3         | 735.371  | 38.91                | 4.1   | 62.9   | x               | x                 | x               | 1  |
| 95  | 80         | 98       | HIQKEDVPSERYLGYLEQL       | none         | 3         | 773.065  | 50.14                | 4.1   | 58.0   | x               | x                 | x               | 1  |
| 96  | 80         | 99       | HIQKEDVPSERYLGYLEQLL      | none         | 2 (3)     | 1215.638 | 61.48                | 4.0   | 71.3   | x               | x                 | x               | 5  |
| 97  | 80         | 100      | HIQKEDVPSERYLGYLEQLLR     | none         | 4 (3,5)   | 647.346  | 58.44                | 4.5   | 57.3   | x               | x                 | x               | 1; 3; 5  |
| 98  | 80         | 101      | HIQKEDVPSERYLGYLEQLLRL    | none         | 4 (3)     | 675.618  | 67.03                | 3.9   | 48.5   | x               | x                 | x               |  |
| 99  | 80         | 102      | HIQKEDVPSERYLGYLEQLLRLK   | none         | 5 (3,4)   | 566.314  | 60.64                | 4.5   | 57.2   | x               | x                 | x               | 1; 3; 5  |
| 100 | 80         | 103      | HIQKEDVPSERYLGYLEQLLRLKK  | none         | 3 (4,5,6) | 985.888  | 56.22                | 3.2   | 28.2   | x               | x                 | x               | 1  |
| 101 | 80         | 104      | HIQKEDVPSERYLGYLEQLLRLKKY | none         | 5         | 624.547  | 57.25                | 4.0   | 39.7   | x               | x                 | x               |  |
| 102 | 81         | 89       | IQKEDVPSE                 | none         | 2         | 522.762  | 17.04                | 2.2   | 36.3   | x               | x                 | x               | 1; 3; 5  |
| 103 | 81         | 90       | IQKEDVPSER                | none         | 2 (3)     | 400.878  | 15.15                | 2.9   | 54.6   | x               | x                 | x               | 1; 3; 5  |
| 104 | 81         | 91       | IQKEDVPSERY               | none         | 2         | 682.345  | 21.29                | 2.7   | 50.6   | x               | x                 | x               | 5  |
| 105 | 81         | 92       | IQKEDVPSERYL              | none         | 3         | 492.927  | 29.90                | 3.1   | 50.6   | x               | x                 | x               | 1  |
| 106 | 81         | 93       | IQKEDVPSERYLG             | none         | 3         | 511.934  | 28.05                | 2.8   | 37.5   | x               | x                 | x               | 1  |
| 107 | 82         | 93       | QKEDVPSERYLG              | none         | 3 (2)     | 474.240  | 25.15                | 2.6   | 27.4   | x               | x                 |                 | 1  |
| 108 | 83         | 91       | KEDVPSERY                 | none         | 2         | 561.773  | 17.22                | 3.1   | 46.1   | x               | x                 | x               | 1; 5   |
| 109 | 83         | 93       | KEDVPSERYLG               | none         | 2         | 646.827  | 24.93                | 2.8   | 54.4   | x               | x                 |                 | 1  |
| 110 | 84         | 91       | EDVPSERY                  | none         | 2         | 497.727  | 20.58                | 1.4   | 46.9   | x               | x                 | x               |  |
| 111 | 86         | 97       | VPSERYLGYLEQ              | none         | 2         | 727.370  | 40.77                | 2.2   | 47.0   | x               | x                 | x               | 1  |

| Nr. | Start pos. | End pos. | Sequence                          | Modification | z       | m/z     | t <sub>r</sub> (min) | Xcorr | -10lgP | RM <sup>a</sup> | UH T <sup>a</sup> | IF <sup>a</sup> | Literature (milk <sup>1-6</sup> , colostrum <sup>7</sup> ) |
|-----|------------|----------|-----------------------------------|--------------|---------|---------|----------------------|-------|--------|-----------------|-------------------|-----------------|--|
| 112 | 86         | 98       | VPSERYLGYLEQL                     | none         | 2       | 783.911 | 53.16                | 2.7   | 58.0   | x               | x                 | x               | 1  |
| 113 | 86         | 99       | VPSERYLGYLEQLL                    | none         | 2       | 840.453 | 65.13                | 2.6   | 51.1   | x               | x                 | x               | 1  |
| 114 | 91         | 99       | YLGYLEQLL                         | none         | 2       | 556.304 | 64.78                | 1.5   | 24.2   | x               | x                 | x               | 5  |
| 115 | 91         | 100      | YLGYLEQLLR                        | none         | 2       | 634.355 | 58.27                | 3.3   | 67.7   | x               | x                 | x               |  |
| 116 | 91         | 102      | YLGYLEQLLRLK                      | none         | 2 (3)   | 754.945 | 60.51                | 3.8   | 68.5   | x               | x                 | x               |  |
| 117 | 91         | 103      | YLGYLEQLLRLKK                     | none         | 3 (4)   | 546.330 | 54.07                | 2.5   | 36.5   | x               | x                 | x               |  |
| 118 | 92         | 100      | LGYLEQLLR                         | none         | 2       | 552.823 | 51.92                | 3.2   | 55.6   | x               | x                 | x               | 1; 3; 5  |
| 119 | 92         | 102      | LGYLEQLLRLK                       | none         | 3       | 449.278 | 55.65                | 3.0   | 56.8   | x               | x                 | x               |  |
| 120 | 93         | 99       | GYLEQLL                           | none         | 2       | 418.231 | 53.87                | 1.8   | 34.9   | x               | x                 | x               |  |
| 121 | 93         | 100      | GYLEQLLR                          | none         | 2       | 496.281 | 46.78                | 2.6   | 50.9   | x               | x                 | x               | 1  |
| 122 | 93         | 101      | GYLEQLLRL                         | none         | 2       | 552.823 | 61.34                | 2.1   | 44.7   | x               | x                 | x               | 5  |
| 123 | 93         | 102      | GYLEQLLRLK                        | none         | 2 (3)   | 616.871 | 51.98                | 3.4   | 58.7   | x               | x                 | x               | 5  |
| 124 | 94         | 100      | YLEQLLR                           | none         | 2       | 467.771 | 39.11                | 2.6   | 39.9   | x               | x                 | x               | 1; 5   |
| 125 | 94         | 101      | YLEQLLRL                          | none         | 2       | 524.312 | 54.57                | 2.5   | 38.1   | x               | x                 | x               | 1  |
| 126 | 94         | 102      | YLEQLLRLK                         | none         | 2       | 588.360 | 44.78                | 2.8   | 49.6   | x               | x                 | x               | 1  |
| 127 | 95         | 101      | LEQLLRL                           | none         | 2       | 442.782 | 45.15                | 2.3   | 32.2   | x               | x                 | x               | 1  |
| 128 | 95         | 102      | LEQLLRLK                          | none         | 2       | 506.828 | 34.31                | 3.0   | 36.8   | x               | x                 | x               | 1  |
| 129 | 101        | 123      | LKKYKVPQLEIVPNsAEERLHSM           | S15(Phospho) | 3 (4,5) | 930.486 | 43.25                | 5.4   | 62.6   | x               | x                 | x               | 5  |
| 130 | 103        | 119      | KYKVPQLEIVPNsAEEER                | none         | 3       | 667.365 | 36.59                | 3.4   | 50.4   | x               | x                 | x               | 3; 5   |
| 131 | 103        | 119      | KYKVPQLEIVPNsAEER                 | S13(Phospho) | 3 (2)   | 694.021 | 38.01                | 4.7   | 62.6   | x               | x                 | x               | 1; 3; 5  |
| 132 | 103        | 121      | KYKVPQLEIVPNsAEERLH               | S13(Phospho) | 4       | 583.304 | 40.08                | 4.4   | 40.6   | x               | x                 | x               |  |
| 133 | 103        | 122      | KYKVPQLEIVPNsAEERLHS              | S13(Phospho) | 4 (3)   | 605.061 | 40.30                | 4.3   | 27.0   | x               | x                 | x               |  |
| 134 | 103        | 123      | KYKVPQLEIVPNsAEERLHSM             | none         | 3 (4)   | 823.437 | 42.87                | 5.0   | 56.7   | x               | x                 | x               | 5  |
| 135 | 103        | 123      | KYKVPQLEIVPNsAEERLHS <sub>m</sub> | M21(Ox)      | 4       | 621.827 | 38.29                | 4.3   | 42.2   | x               | x                 | x               |  |
| 136 | 103        | 123      | KYKVPQLEIVPNsAEERLHSM             | S13(Phospho) | 3 (2,4) | 855.424 | 44.86                | 5.5   | 56.3   | x               | x                 | x               | 5  |
| 137 | 103        | 124      | KYKVPQLEIVPNsAEERLHSMK            | S13(Phospho) | 4 (5)   | 669.844 | 40.83                | 4.4   | 23.3   | x               | x                 | x               | 3; 5   |
| 138 | 104        | 114      | YKVPQLEIVPN                       | none         | 2       | 650.369 | 43.92                | 2.6   | 69.9   |                 |                   | x               |  |
| 139 | 104        | 119      | YKVPQLEIVPNsAEEER                 | none         | 2 (3)   | 936.497 | 40.61                | 4.1   | 78.7   | x               | x                 | x               | 5  |
| 140 | 104        | 119      | YKVPQLEIVPNsAEER                  | S12(Phospho) | 2 (3)   | 976.481 | 42.23                | 5.6   | 77.4   | x               | x                 | x               | 1; 3; 5  |

| Nr. | Start pos. | End pos. | Sequence                     | Modification | z       | m/z      | t <sub>r</sub> (min) | Xcorr | -10lgP | RM <sup>a</sup> | UH T <sup>a</sup> | IF <sup>a</sup> | Literature (milk <sup>1-6</sup> , colostrum <sup>7</sup> ) |
|-----|------------|----------|------------------------------|--------------|---------|----------|----------------------|-------|--------|-----------------|-------------------|-----------------|--|
| 141 | 104        | 122      | YKVPQLEIVPNsAEERLHS          | S12(Phospho) | 3       | 763.714  | 43.72                | 4.7   | 48.8   | x               | x                 | x               | 5  |
| 142 | 104        | 123      | YKVPQLEIVPNSAEERLHSM         | none         | 3 (4)   | 780.740  | 46.08                | 3.8   | 55.8   | x               | x                 | x               | 5  |
| 143 | 104        | 123      | YKVPQLEIVPNSAEERLHSm         | M20(Ox)      | 3       | 786.071  | 41.64                | 3.7   | 58.3   | x               | x                 | x               | 3  |
| 144 | 104        | 123      | YKVPQLEIVPNsAEERLHSM         | S12(Phospho) | 3 (2,4) | 807.394  | 48.27                | 4.7   | 56.7   | x               | x                 | x               | 1; 3; 5  |
| 145 | 104        | 124      | YKVPQLEIVPNsAEERLHSMK        | S12(Phospho) | 3 (4)   | 850.091  | 43.88                | 5.0   | 50.6   | x               | x                 | x               | 3; 5   |
| 146 | 105        | 114      | KVPQLEIVPN                   | none         | 2       | 568.837  | 38.05                | 1.6   | 46.1   |                 |                   | x               |  |
| 147 | 105        | 119      | KVPQLEIVPNSAER               | none         | 3       | 570.312  | 35.01                | 4.3   | 62.0   | x               | x                 | x               | 1  |
| 148 | 105        | 119      | KVPQLEIVPNsAER               | S11(Phospho) | 2 (3)   | 894.949  | 37.14                | 4.0   | 41.8   | x               | x                 | x               | 3; 5   |
| 149 | 105        | 121      | KVPQLEIVPNsAEERLH            | S11(Phospho) | 3       | 680.350  | 39.51                | 4.3   | 40.3   |                 |                   | x               |  |
| 150 | 105        | 123      | KVPQLEIVPNSAEERLHSM          | none         | 3       | 726.384  | 42.75                | 5.2   | 57.1   | x               | x                 | x               | 5; 7   |
| 151 | 105        | 123      | KVPQLEIVPNSAEERLHSm          | M19(Ox)      | 3       | 731.715  | 37.46                | 4.2   | 59.0   | x               | x                 | x               | 7  |
| 152 | 105        | 123      | KVPQLEIVPNsAEERLHSM          | S11(Phospho) | 3 (2)   | 753.040  | 45.20                | 5.5   | 50.4   | x               | x                 | x               |  |
| 153 | 105        | 124      | KVPQLEIVPNsAEERLHSMK         | S11(Phospho) | 4       | 597.057  | 40.50                | 2.9   | 24.5   | x               | x                 | x               |  |
| 154 | 106        | 119      | VPQLEIVPNSAER                | none         | 2 (3)   | 790.917  | 38.22                | 3.9   | 86.8   | x               | x                 | x               | 1; 3; 5  |
| 155 | 106        | 119      | VPQLEIVPNsAER                | S10(Phospho) | 2       | 830.901  | 40.32                | 4.7   | 67.8   | x               | x                 | x               | 1; 3; 5  |
| 156 | 106        | 121      | VPQLEIVPNsAEERLH             | S10(Phospho) | 3 (2)   | 637.652  | 42.59                | 4.5   | 47.6   | x               | x                 | x               |  |
| 157 | 106        | 122      | VPQLEIVPNSAEERLHS            | none         | 3       | 640.007  | 40.51                | 3.5   | 40.5   | x               | x                 | x               | 1; 5   |
| 158 | 106        | 122      | VPQLEIVPNsAEERLHS            | S10(Phospho) | 2 (3)   | 999.488  | 42.66                | 4.7   | 59.0   | x               | x                 | x               |  |
| 159 | 106        | 123      | VPQLEIVPNSAEERLHSM           | none         | 3 (2)   | 683.685  | 45.68                | 4.8   | 89.8   | x               | x                 | x               | 5  |
| 160 | 106        | 123      | VPQLEIVPNSAEERLHSm           | M18(Ox)      | 3 (2)   | 689.017  | 40.08                | 4.9   | 84.4   | x               | x                 | x               |  |
| 161 | 106        | 123      | VPQLEIVPNsAEERLHSM           | S10(Phospho) | 3 (2)   | 710.342  | 48.28                | 5.4   | 73.3   | x               | x                 | x               | 3; 5   |
| 162 | 106        | 124      | VPQLEIVPNsAEERLHSMK          | none         | 3       | 726.383  | 41.19                | 3.3   | 37.6   | x               | x                 | x               |  |
| 163 | 106        | 124      | VPQLEIVPNsAEERLHSMK          | S10(Phospho) | 2 (3,4) | 1129.056 | 42.96                | 4.4   | 66.1   | x               | x                 | x               | 5  |
| 164 | 106        | 131      | VPQLEIVPNsAEERLHSMSKEGIHAQQ  | S10(Phospho) | 3       | 1007.494 | 43.59                | 4.8   | 34.5   | x               | x                 | x               |  |
| 165 | 106        | 132      | VPQLEIVPNsAEERLHSMSKEGIHAQQK | S10(Phospho) | 4 (5)   | 630.518  | 41.32                | 3.8   | 23.0   | x               | x                 | x               |  |
| 166 | 108        | 119      | QLEIVPNSAER                  | none         | 2       | 692.855  | 31.41                | 2.4   | 62.7   | x               | x                 | x               | 5  |
| 167 | 108        | 119      | QLEIVPNsAER                  | S8(Phospho)  | 2       | 732.840  | 33.73                | 2.9   | 54.2   | x               | x                 | x               | 1; 3; 5  |
| 168 | 108        | 123      | QLEIVPNSAEERLHSM             | none         | 3       | 618.312  | 41.19                | 2.9   | 41.1   | x               | x                 | x               |  |
| 169 | 108        | 123      | QLEIVPNsAEERLHSM             | S8(Phospho)  | 3 (2)   | 644.967  | 44.50                | 2.7   | 28.1   | x               | x                 | x               |  |

| Nr. | Start pos. | End pos. | Sequence                            | Modification | z     | m/z      | t <sub>r</sub> (min) | Xcorr | -10lgP | RM <sup>a</sup> | UH T <sup>a</sup> | IF <sup>a</sup> | Literature (milk <sup>1-6</sup> , colostrum <sup>7</sup> ) |
|-----|------------|----------|-------------------------------------|--------------|-------|----------|----------------------|-------|--------|-----------------|-------------------|-----------------|--|
| 170 | 108        | 124      | QLEIVPNsAEERLHSMK                   | S8(Phospho)  | 3     | 687.667  | 39.02                | 2.5   | 23.3   | x               | x                 | x               | 5  |
| 171 | 109        | 119      | LEIVPNSAER                          | none         | 2     | 628.827  | 29.74                | 2.7   | 56.5   | x               | x                 | x               | 1; 5   |
| 172 | 109        | 119      | LEIVPNSAER                          | S7(Phospho)  | 2     | 668.809  | 32.06                | 2.8   | 45.2   | x               | x                 | x               | 1; 5   |
| 173 | 109        | 123      | LEIVPNSAEERLHSM                     | S7(Phospho)  | 2     | 902.919  | 43.78                | 3.5   | 57.5   | x               | x                 |                 |  |
| 174 | 110        | 119      | EIVPNSAER                           | none         | 2     | 572.284  | 20.14                | 1.9   | 40.4   | x               | x                 | x               | 1; 5   |
| 175 | 110        | 119      | EIVPNSAER                           | S6(Phospho)  | 2     | 612.268  | 22.13                | 2.2   | 47.2   | x               | x                 | x               | 5  |
| 176 | 111        | 123      | IVPNsAEERLHSM                       | S5(Phospho)  | 2     | 781.856  | 33.02                | 2.8   | 35.6   | x               | x                 | x               |  |
| 177 | 112        | 123      | VPNsAEERLHSM                        | S4(Phospho)  | 2     | 725.311  | 27.58                | 2.8   | 60.0   | x               | x                 | x               |  |
| 178 | 114        | 123      | NsAEERLHSM                          | S2(Phospho)  | 2     | 627.252  | 23.47                | 1.8   | 46.0   | x               | x                 |                 | 5  |
| 179 | 115        | 123      | SAEERLHSM                           | none         | 2     | 530.247  | 17.95                | 1.9   | 58.6   |                 |                   | x               |  |
| 180 | 115        | 123      | sAEERLHSM                           | S1(Phospho)  | 2     | 570.230  | 19.99                | 2.7   | 45.3   |                 |                   | x               |  |
| 181 | 125        | 144      | EGIHAQQKEPMIGVNQELAY                | none         | 3     | 752.377  | 39.50                | 2.9   | 46.1   | x               | x                 | x               | 5  |
| 182 | 125        | 150      | EGIHAQQKEPmIGVNQELAYFYPELF          | M11(Ox)      | 3     | 1023.168 | 63.21                | 2.7   | 22.5   | x               | x                 |                 |  |
| 183 | 131        | 144      | QKEPMIGVNQELAY                      | none         | 2     | 810.411  | 40.43                | 2.5   | 72.3   |                 |                   | x               |  |
| 184 | 132        | 144      | KEPMIGVNQELAY                       | none         | 2     | 746.380  | 40.35                | 2.9   | 65.4   |                 |                   | x               |  |
| 185 | 145        | 154      | FYPELFRQFY                          | none         | 2     | 705.348  | 58.74                | 2.2   | 55.3   | x               | x                 | x               | 5  |
| 186 | 166        | 199      | YVPLGTQYTDAPSFSIDIPNPIGSENSEKTTMPLW | none         | 3     | 1252.600 | 65.31                | 3.4   | 54.3   | x               | x                 | x               | 5  |
| 187 | 166        | 199      | YVPLGTQYTDAPSFSIDIPNPIGSENSEKTTmPLW | M31(Ox)      | 3     | 1257.929 | 62.01                | 4.5   | 52.1   | x               | x                 | x               | 5  |
| 188 | 171        | 199      | TQYTDAPSFSIDIPNPIGSENSEKTTmPLW      | M26(Ox)      | 3     | 1081.500 | 57.92                | 3.5   | 42.8   |                 |                   | x               |  |
| 189 | 172        | 194      | QYTDAPSFSIDIPNPIGSENSEKT            | none         | 2     | 1249.073 | 47.31                | 3.5   | 61.6   | x               | x                 | x               |  |
| 190 | 172        | 199      | QYTDAPSFSIDIPNPIGSENSEKTTMPLW       | none         | 3 (2) | 1042.486 | 61.70                | 3.4   | 66.4   | x               | x                 | x               |  |
| 191 | 172        | 199      | QYTDAPSFSIDIPNPIGSENSEKTTmPLW       | M25(Ox)      | 3 (2) | 1047.818 | 57.99                | 4.0   | 59.5   | x               | x                 | x               |  |
| 192 | 174        | 197      | TDAPSFSIDIPNPIGSENSEKTTMP           | none         | 2     | 1268.082 | 49.71                | 3.0   | 50.8   | x               | x                 | x               | 5; 7   |
| 193 | 174        | 199      | TDAPSFSIDIPNPIGSENSEKTTMPLW         | none         | 2 (3) | 1417.666 | 60.94                | 3.2   | 67.1   | x               | x                 | x               | 5  |
| 194 | 174        | 199      | TDAPSFSIDIPNPIGSENSEKTTmPLW         | M23(Ox)      | 3 (2) | 950.777  | 57.11                | 3.6   | 69.4   | x               | x                 | x               | 5  |
| 195 | 176        | 190      | APSFSDIPNPIGSEN                     | none         | 2     | 772.865  | 47.97                | 3.0   | 66.6   |                 |                   | x               |  |
| 196 | 176        | 193      | APSFSDIPNPIGSENSEK                  | none         | 2     | 944.951  | 43.49                | 4.7   | 78.3   | x               | x                 | x               |  |
| 197 | 176        | 199      | APSFSDIPNPIGSENSEKTTMPLW            | none         | 2     | 1309.627 | 59.81                | 4.6   | 94.1   | x               | x                 | x               | 1; 5; 6  |
| 198 | 176        | 199      | APSFSDIPNPIGSENSEKTTmPLW            | M21(Ox)      | 2     | 1317.626 | 56.21                | 4.2   | 86.6   | x               | x                 | x               | 3  |

| Nr. | Start pos. | End pos. | Sequence                | Modification | z     | m/z      | t <sub>r</sub> (min) | Xcorr | -10lgP | RM <sup>a</sup> | UH T <sup>a</sup> | IF <sup>a</sup> | Literature (milk <sup>1-6</sup> , colostrum <sup>7</sup> ) |
|-----|------------|----------|-------------------------|--------------|-------|----------|----------------------|-------|--------|-----------------|-------------------|-----------------|--|
| 199 | 177        | 199      | PSFSDIPNPIGSENSEKTTMPLW | none         | 2     | 1274.110 | 59.48                | 3.5   | 74.3   |                 | x                 |                 |  |
| 200 | 177        | 199      | PSFSDIPNPIGSENSEKTTmPLW | M20(Ox)      | 2     | 1282.107 | 55.39                | 3.2   | 57.2   |                 | x                 |                 |  |
| 201 | 178        | 199      | SFSDIPNPIGSENSEKTTMPLW  | none         | 2     | 1225.582 | 58.20                | 3.8   | 82.7   | x               | x                 | x               |  |
| 202 | 178        | 199      | SFSDIPNPIGSENSEKTTmPLW  | M19(Ox)      | 2 (3) | 1233.580 | 53.81                | 3.7   | 76.0   | x               | x                 | x               |  |
| 203 | 179        | 199      | FSDIPNPIGSENSEKTTMPLW   | none         | 2     | 1182.068 | 56.90                | 4.0   | 78.2   | x               | x                 | x               | 5  |
| 204 | 179        | 199      | FSDIPNPIGSENSEKTTmPLW   | M18(Ox)      | 2     | 1190.061 | 52.31                | 3.7   | 82.9   |                 | x                 |                 |  |
| 205 | 180        | 193      | SDIPNPIGSENSEK          | none         | 2     | 743.853  | 29.93                | 2.2   | 53.4   | x               | x                 |                 | 5  |
| 206 | 180        | 194      | SDIPNPIGSENSEKT         | none         | 2     | 794.379  | 30.65                | 3.7   | 73.9   | x               | x                 | x               |  |
| 207 | 180        | 197      | SDIPNPIGSENSEKTTMP      | none         | 2     | 958.950  | 38.11                | 2.3   | 61.5   | x               | x                 | x               | 1; 5; 7  |
| 208 | 180        | 197      | SDIPNPIGSENSEKTTmP      | M17(Ox)      | 2     | 966.946  | 32.71                | 4.4   | 71.7   | x               | x                 | x               | 1; 5; 7  |
| 209 | 180        | 198      | SDIPNPIGSENSEKTTMPL     | none         | 2     | 1015.493 | 44.62                | 3.2   | 54.4   | x               | x                 | x               |  |
| 210 | 180        | 199      | SDIPNPIGSENSEKTTMPLW    | none         | 2 (3) | 1108.531 | 53.03                | 4.2   | 99.0   | x               | x                 | x               | 1; 2; 5  |
| 211 | 180        | 199      | SDIPNPIGSENSEKTTmPLW    | M17(Ox)      | 2 (3) | 1116.529 | 48.45                | 4.3   | 98.7   | x               | x                 | x               | 1; 2; 5  |
| 212 | 181        | 197      | DIPNPIGSENSEKTTMP       | none         | 2     | 915.434  | 39.17                | 2.7   | 52.4   | x               | x                 | x               | 1; 5   |
| 213 | 181        | 197      | DIPNPIGSENSEKTTmP       | M16(Ox)      | 2     | 923.429  | 33.43                | 3.0   | 50.8   | x               | x                 | x               | 1; 5   |
| 214 | 181        | 199      | DIPNPIGSENSEKTTMPLW     | none         | 2     | 1065.015 | 54.84                | 3.9   | 78.7   | x               | x                 | x               | 1; 5   |
| 215 | 181        | 199      | DIPNPIGSENSEKTTmPLW     | M16(Ox)      | 2     | 1073.012 | 50.01                | 3.8   | 88.1   | x               | x                 | x               |  |
| 216 | 182        | 193      | IPNPIGSENSEK            | none         | 2     | 642.826  | 25.99                | 2.7   | 52.1   |                 | x                 |                 |  |
| 217 | 182        | 197      | IPNPIGSENSEKTTMP        | none         | 2     | 857.920  | 35.69                | 4.5   | 56.0   | x               | x                 | x               | 1; 2; 5  |
| 218 | 182        | 197      | IPNPIGSENSEKTTmP        | M15(Ox)      | 2     | 865.916  | 29.42                | 4.5   | 55.1   | x               | x                 | x               | 1  |
| 219 | 182        | 199      | IPNPIGSENSEKTTMPLW      | none         | 2     | 1007.501 | 51.48                | 4.4   | 100.8  | x               | x                 | x               | 1; 4; 5  |
| 220 | 182        | 199      | IPNPIGSENSEKTTmPLW      | M15(Ox)      | 2     | 1015.499 | 46.94                | 4.9   | 98.0   | x               | x                 | x               | 1  |
| 221 | 182        | 199      | IPNPIGsENSEKTTMPLW      | S7(Phospho)  | 2     | 1047.486 | 55.91                | 4.6   | 52.4   |                 | x                 |                 |  |
| 222 | 183        | 199      | PNPIGSENSEKTTMPLW       | none         | 2     | 950.959  | 60.00                | 2.4   | 66.2   | x               | x                 | x               |  |
| 223 | 183        | 199      | PNPIGSENSEKTTmPLW       | M14(Ox)      | 2     | 958.955  | 56.06                | 3.3   | 65.1   | x               | x                 | x               |  |
| 224 | 184        | 197      | NPIGSENSEKTTMP          | none         | 2     | 752.851  | 25.82                | 2.2   | 46.8   | x               |                   | x               | 1; 7   |
| 225 | 184        | 197      | NPIGSENSEKTTmP          | M13(Ox)      | 2     | 760.848  | 19.12                | 2.3   | 58.0   | x               | x                 | x               | 5  |
| 226 | 184        | 199      | NPIGSENSEKTTMPLW        | none         | 2     | 902.435  | 45.67                | 3.6   | 87.8   | x               | x                 | x               |  |
| 227 | 184        | 199      | NPIGSENSEKTTmPLW        | M13(Ox)      | 2     | 910.431  | 38.94                | 4.0   | 89.7   | x               | x                 | x               |  |

| Nr.                             | Start pos. | End pos. | Sequence                | Modification | z     | m/z     | t <sub>r</sub> (min) | Xcorr | -10lgP | RM <sup>a</sup> | UH T <sup>a</sup> | IF <sup>a</sup> | Literature (milk <sup>1-6</sup> , colostrum <sup>7</sup> ) |
|---------------------------------|------------|----------|-------------------------|--------------|-------|---------|----------------------|-------|--------|-----------------|-------------------|-----------------|--|
| 228                             | 185        | 197      | PIGSENSEKTTMP           | none         | 2     | 695.826 | 23.71                | 3.0   | 56.9   | x               | x                 | x               | 1; 3; 5  |
| 229                             | 185        | 197      | PIGSENSEKTTmP           | M12(Ox)      | 2     | 703.826 | 16.47                | 3.3   | 62.3   | x               | x                 | x               | 3  |
| 230                             | 185        | 198      | PIGSENSEKTTmPL          | M12(Ox)      | 2     | 760.369 | 24.90                | 2.4   | 52.5   |                 | x                 |                 |  |
| 231                             | 185        | 199      | PIGSENSEKTTMPLW         | none         | 2     | 845.412 | 45.26                | 4.0   | 103.5  | x               | x                 | x               | 1; 4; 6  |
| 232                             | 185        | 199      | PIGSENSEKTTmPLW         | M12(Ox)      | 2     | 853.410 | 38.98                | 3.7   | 96.8   | x               | x                 | x               |  |
| 233                             | 185        | 199      | PIGsENSEKTTMPLW         | S4(Phospho)  | 2     | 885.395 | 49.91                | 3.2   | 64.1   |                 | x                 |                 |  |
| 234                             | 186        | 197      | IGSENSEKTTMP            | none         | 2     | 647.302 | 21.38                | 1.8   | 52.1   | x               | x                 | x               |  |
| 235                             | 186        | 199      | IGSENSEKTTMPLW          | none         | 2     | 796.886 | 43.86                | 2.9   | 73.8   | x               | x                 | x               |  |
| 236                             | 186        | 199      | IGSENSEKTTmPLW          | M11(Ox)      | 2     | 804.884 | 36.41                | 2.8   | 63.7   | x               | x                 | x               |  |
| 237                             | 188        | 199      | SENSEKTTMPLW            | none         | 2     | 711.833 | 41.59                | 3.2   | 66.1   | x               | x                 | x               |  |
| 238                             | 188        | 199      | SENSEKTTmPLW            | M9(Ox)       | 2     | 719.829 | 33.19                | 2.8   | 67.6   | x               | x                 | x               |  |
| 239                             | 189        | 199      | ENSEKTTMPLW             | none         | 2     | 668.316 | 41.90                | 2.2   | 58.9   |                 | x                 | x               |  |
| 240                             | 189        | 199      | ENSEKTTmPLW             | M8(Ox)       | 2     | 676.313 | 33.41                | 2.7   | 49.0   |                 | x                 | x               |  |
| 241                             | 190        | 199      | NSEKTTMPLW              | none         | 2     | 603.793 | 41.04                | 2.6   | 58.7   |                 | x                 |                 |  |
| 242                             | 190        | 199      | NSEKTTmPLW              | M7(Ox)       | 2     | 611.791 | 32.42                | 2.3   | 56.9   |                 | x                 |                 |  |
| 243                             | 191        | 199      | SEKTTMPLW               | none         | 2     | 546.773 | 41.20                | 2.1   | 47.5   | x               | x                 | x               | 1  |
| 244                             | 191        | 199      | SEKTTmPLW               | M6(Ox)       | 2     | 554.770 | 32.54                | 2.5   | 49.9   | x               | x                 | x               |  |
| 245                             | 192        | 199      | EKTTMPLW                | none         | 2     | 503.257 | 41.54                | 1.0   | 44.0   |                 | x                 |                 |  |
| 246                             | 193        | 199      | KTTMPLW                 | none         | 2     | 438.735 | 40.39                | 1.7   | 40.2   |                 | x                 |                 |  |
| <b>Alpha-S2-casein (P02663)</b> |            |          |                         |              |       |         |                      |       |        |                 |                   |                 |  |
| 247                             | 1          | 20       | KNTMEHVSSEESIISQETY     | none         | 3     | 767.017 | 35.33                | 4.1   | 36.9   | x               | x                 | x               | 5  |
| 248                             | 1          | 20       | KNTmEHVSSEESIISQETY     | M4(Ox)       | 3     | 772.349 | 31.91                | 4.2   | 44.4   | x               | x                 | x               |  |
| 249                             | 1          | 21       | KNTMEHVSSEESIISQETYK    | none         | 3 (4) | 809.715 | 32.13                | 7.3   | 84.3   | x               | x                 | x               | 5  |
| 250                             | 1          | 21       | KNTmEHVSSEESIISQETYK    | M4(Ox)       | 3 (4) | 815.049 | 28.41                | 5.7   | 60.9   | x               | x                 | x               |  |
| 251                             | 1          | 21       | KNTMEHVSSEESIIsQETYK    | S16(Phospho) | 3     | 836.371 | 33.11                | 7.4   | 86.0   | x               | x                 | x               | 5  |
| 252                             | 1          | 23       | KNTMEHVSSEESIISQETYKQE  | none         | 3     | 895.417 | 32.58                | 3.9   | 50.2   | x               | x                 | x               |  |
| 253                             | 1          | 24       | KNTMEHVSSEESIISQETYKQEK | none         | 3 (4) | 938.119 | 30.37                | 7.1   | 69.4   | x               | x                 | x               | 1; 3; 5  |
| 254                             | 1          | 24       | KNTmEHVSSEESIISQETYKQEK | M4(Ox)       | 4 (3) | 707.836 | 26.64                | 6.1   | 59.5   | x               | x                 | x               | 5  |
| 255                             | 1          | 24       | KNTMEHVSSEESIIsQETYKQEK | S16(Phospho) | 3 (4) | 964.769 | 31.28                | 6.3   | 63.9   | x               | x                 | x               | 3; 5   |

| Nr. | Start pos. | End pos. | Sequence           | Modification | z     | m/z     | t <sub>r</sub> (min) | Xcorr | -10lgP | RM <sup>a</sup> | UH T <sup>a</sup> | IF <sup>a</sup> | Literature (milk <sup>1-6</sup> , colostrum <sup>7</sup> ) |
|-----|------------|----------|--------------------|--------------|-------|---------|----------------------|-------|--------|-----------------|-------------------|-----------------|--|
| 256 | 9          | 21       | SSEESIISQETYK      | none         | 2     | 750.858 | 30.66                | 3.1   | 58.6   | x               | x                 | x               |  |
| 257 | 11         | 21       | EESIIsQETYK        | S6(Phospho)  | 2     | 703.808 | 32.97                | 2.7   | 51.5   |                 |                   | x               |  |
| 258 | 13         | 21       | SIIIsQETYK         | S4(Phospho)  | 2     | 574.766 | 31.64                | 2.7   | 31.0   |                 |                   | x               |  |
| 259 | 14         | 21       | IIsQETYK           | S3(Phospho)  | 2     | 531.248 | 24.15                | 3.2   | 43.2   | x               | x                 | x               | 5  |
| 260 | 14         | 22       | IIsQETYKQ          | S3(Phospho)  | 2     | 595.275 | 24.14                | 2.7   | 46.8   | x               | x                 |                 | 5  |
| 261 | 14         | 24       | IIsQETYKQEK        | S3(Phospho)  | 2     | 723.847 | 20.93                | 2.3   | 45.8   | x               | x                 | x               |  |
| 262 | 71         | 78       | ITVDDKHY           | none         | 2     | 495.747 | 19.35                | 2.2   | 51.7   | x               | x                 | x               |  |
| 263 | 71         | 79       | ITVDDKHYQ          | none         | 2     | 559.777 | 18.20                | 2.2   | 51.1   | x               | x                 | x               | 1  |
| 264 | 81         | 88       | ALNEINQF           | none         | 2     | 474.743 | 38.83                | 2.4   | 45.0   |                 |                   | x               |  |
| 265 | 81         | 89       | ALNEINQFY          | none         | 2     | 556.274 | 45.06                | 2.3   | 47.6   |                 |                   | x               |  |
| 266 | 81         | 95       | ALNEINQFYQKFPQY    | none         | 2     | 951.975 | 52.32                | 2.9   | 56.6   |                 |                   | x               |  |
| 267 | 81         | 98       | ALNEINQFYQKFPQYLQY | none         | 3 (2) | 769.721 | 59.86                | 4.4   | 59.7   |                 |                   | x               | 5  |
| 268 | 88         | 98       | FYQKFPQYLQY        | none         | 2     | 762.880 | 46.64                | 3.0   | 50.0   |                 |                   | x               |  |
| 269 | 89         | 95       | YQKFPQY            | none         | 2     | 487.242 | 28.61                | 2.2   | 52.2   |                 |                   | x               |  |
| 270 | 89         | 98       | YQKFPQYLQY         | none         | 2     | 689.348 | 42.20                | 3.1   | 64.3   |                 |                   | x               |  |
| 271 | 90         | 98       | QKFPQYLQY          | none         | 2     | 607.814 | 39.81                | 2.6   | 53.9   |                 |                   | x               |  |
| 272 | 98         | 113      | YLYQGPIVLNPWDQVK   | none         | 2     | 967.015 | 56.97                | 4.0   | 71.2   | x               | x                 |                 | 5  |
| 273 | 99         | 113      | LYQGPIVLNPWDQVK    | none         | 3 (2) | 590.658 | 53.44                | 4.4   | 80.9   | x               | x                 | x               | 7  |
| 274 | 99         | 114      | LYQGPIVLNPWDQVKR   | none         | 2 (3) | 963.535 | 48.82                | 3.8   | 95.6   | x               | x                 | x               |  |
| 275 | 99         | 115      | LYQGPIVLNPWDQVKRN  | none         | 2 (3) | 680.707 | 48.62                | 3.3   | 46.4   |                 |                   | x               |  |
| 276 | 100        | 112      | YQGPIVLNPWDQV      | none         | 2     | 764.895 | 58.72                | 3.0   | 41.4   |                 |                   | x               | 7  |
| 277 | 100        | 113      | YQGPIVLNPWDQVK     | none         | 2     | 828.941 | 50.57                | 3.8   | 75.3   | x               | x                 | x               | 7  |
| 278 | 100        | 114      | YQGPIVLNPWDQVKR    | none         | 3     | 604.996 | 45.97                | 3.5   | 79.5   | x               | x                 | x               |  |
| 279 | 100        | 115      | YQGPIVLNPWDQVKRN   | none         | 3     | 643.011 | 45.69                | 1.8   | 42.7   |                 |                   | x               |  |
| 280 | 101        | 113      | QGPIVLNPWDQVK      | none         | 2     | 747.409 | 47.66                | 2.8   | 63.9   | x               | x                 | x               | 5  |
| 281 | 101        | 114      | QGPIVLNPWDQVKR     | none         | 3     | 550.643 | 42.99                | 2.7   | 42.9   | x               | x                 | x               |  |
| 282 | 102        | 112      | GPIVLPNPDQV        | none         | 2     | 619.333 | 55.93                | 2.1   | 36.4   | x               |                   |                 | 5  |
| 283 | 102        | 113      | GPIVLPNPDQVK       | none         | 2     | 683.379 | 47.32                | 3.4   | 68.6   | x               | x                 | x               | 3; 5   |
| 284 | 105        | 113      | VLPNPDQVK          | none         | 2     | 549.799 | 37.70                | 2.2   | 51.1   | x               | x                 | x               | 1  |

| Nr. | Start pos. | End pos. | Sequence                           | Modification | z     | m/z      | t <sub>r</sub> (min) | Xcorr | -10lgP | RM <sup>a</sup> | UH T <sup>a</sup> | IF <sup>a</sup> | Literature (milk <sup>1-6</sup> , colostrum <sup>7</sup> ) |
|-----|------------|----------|------------------------------------|--------------|-------|----------|----------------------|-------|--------|-----------------|-------------------|-----------------|--|
| 285 | 115        | 128      | NAVPIPTLNREQL                      | none         | 2     | 783.437  | 40.03                | 2.4   | 59.5   |                 | x                 | x               |  |
| 286 | 115        | 135      | NAVPIPTLNREQLSTSEENS               | none         | 2     | 1150.573 | 36.88                | 3.9   | 85.9   | x               | x                 | x               | 1  |
| 287 | 115        | 135      | NAVPIPTLNREQLSTsEENS               | S17(Phospho) | 2     | 1190.556 | 38.62                | 4.1   | 58.5   | x               | x                 | x               |  |
| 288 | 115        | 136      | NAVPIPTLNREQLSTsEENSK              | S17(Phospho) | 2     | 1254.605 | 35.25                | 5.0   | 52.0   | x               | x                 | x               |  |
| 289 | 115        | 149      | NAVPIPTLNREQLSTsEENSKKTVDMESTEVFTK | S17(Phospho) | 3     | 1335.314 | 42.34                | 4.1   | 32.3   | x               | x                 | x               |  |
| 290 | 123        | 135      | LNREQLSTSEENS                      | none         | 2     | 753.854  | 19.61                | 2.8   | 53.8   | x               | x                 | x               |  |
| 291 | 123        | 136      | LNREQLSTsEENSK                     | S9(Phospho)  | 2 (3) | 857.885  | 18.43                | 4.0   | 51.8   | x               | x                 | x               |  |
| 292 | 123        | 137      | LNREQLSTsEENSKK                    | S9(Phospho)  | 3     | 614.957  | 16.25                | 3.2   | 18.9   | x               | x                 | x               |  |
| 293 | 123        | 149      | LNREQLSTsEENSKKTVDMESTEVFTK        | S9(Phospho)  | 4     | 803.377  | 34.35                | 4.9   | 56.4   | x               | x                 | x               | 5  |
| 294 | 135        | 149      | SKKTVDMEsTEVFTK                    | S9(Phospho)  | 3     | 603.948  | 28.30                | 5.7   | 71.5   | x               | x                 | x               |  |
| 295 | 137        | 149      | KTVDMESTEVFTK                      | none         | 2 (3) | 757.873  | 30.56                | 4.4   | 85.5   | x               | x                 | x               | 1; 5   |
| 296 | 137        | 149      | KTVDmESTEVFTK                      | M5(Ox)       | 2     | 510.916  | 23.93                | 2.4   | 42.9   | x               | x                 | x               |  |
| 297 | 137        | 149      | KTVDMEsTEVFTK                      | S7(Phospho)  | 2 (3) | 797.857  | 31.88                | 5.7   | 86.5   | x               | x                 | x               | 1; 3; 4; 5   |
| 298 | 137        | 150      | KTVDMESTEVFTKK                     | none         | 3     | 548.281  | 27.36                | 5.7   | 74.0   | x               | x                 | x               | 3; 5   |
| 299 | 137        | 150      | KTVDMEsTEVFTKK                     | S7(Phospho)  | 2 (3) | 861.905  | 28.46                | 5.1   | 65.3   | x               | x                 | x               | 1; 5   |
| 300 | 138        | 149      | TVDMESTEVFTK                       | none         | 2     | 693.827  | 35.18                | 3.8   | 91.1   | x               | x                 | x               | 1; 3; 5  |
| 301 | 138        | 149      | TVDmESTEVFTK                       | M4(Ox)       | 2     | 701.822  | 27.51                | 3.5   | 76.4   | x               | x                 | x               | 1; 3; 5  |
| 302 | 138        | 149      | TVDMEsTEVFTK                       | S6(Phospho)  | 2     | 733.810  | 36.40                | 4.9   | 75.1   | x               | x                 | x               | 1; 3; 5  |
| 303 | 138        | 150      | TVDmESTEVFTKK                      | M4(Ox)       | 2 (3) | 765.871  | 24.32                | 3.1   | 53.5   | x               | x                 | x               | 3  |
| 304 | 139        | 149      | VDMESTEVFTK                        | none         | 2     | 643.301  | 34.10                | 3.4   | 84.6   | x               | x                 | x               | 5  |
| 305 | 139        | 149      | VDMEsTEVFTK                        | S5(Phospho)  | 2     | 683.286  | 36.36                | 4.6   | 70.1   | x               | x                 | x               | 5  |
| 306 | 139        | 150      | VDMESTEVFTKK                       | none         | 3     | 471.901  | 30.15                | 2.1   | 43.3   | x               | x                 | x               |  |
| 307 | 139        | 150      | VDmESTEVFTKK                       | M3(Ox)       | 3     | 477.232  | 22.39                | 3.1   | 28.7   | x               | x                 | x               |  |
| 308 | 140        | 149      | DmESTEVFTK                         | M2(Ox)       | 2     | 601.764  | 24.01                | 2.7   | 61.1   | x               | x                 | x               |  |
| 309 | 140        | 149      | DMEsTEVFTK                         | S4(Phospho)  | 2     | 633.751  | 33.55                | 3.4   | 56.9   | x               | x                 | x               |  |
| 310 | 141        | 149      | MESTEVFTK                          | none         | 2     | 536.254  | 25.53                | 2.2   | 51.7   | x               | x                 | x               |  |
| 311 | 141        | 149      | MEsTEVFTK                          | S3(Phospho)  | 2     | 576.238  | 28.02                | 3.7   | 56.6   |                 |                   | x               |  |
| 312 | 141        | 150      | MEsTEVFTKK                         | S3(Phospho)  | 2     | 640.285  | 23.57                | 2.8   | 42.9   | x               | x                 | x               |  |
| 313 | 150        | 163      | KTKLTEEKNRLNF                      | none         | 3 (4) | 583.987  | 25.16                | 3.7   | 48.0   | x               | x                 | x               | 1  |

| Nr. | Start pos. | End pos. | Sequence         | Modification | z       | m/z     | t <sub>r</sub> (min) | Xcorr | -10lgP | RM <sup>a</sup> | UH T <sup>a</sup> | IF <sup>a</sup> | Literature (milk <sup>1-6</sup> , colostrum <sup>7</sup> ) |
|-----|------------|----------|------------------|--------------|---------|---------|----------------------|-------|--------|-----------------|-------------------|-----------------|--|
| 314 | 150        | 165      | KTKLTEEEKNRLNFLK | none         | 3 (2,4) | 664.379 | 28.24                | 3.6   | 48.2   | x               | x                 | x               |  |
| 315 | 151        | 161      | TKLTEEEKNRL      | none         | 3       | 454.251 | 19.23                | 2.9   | 48.3   | x               | x                 | x               |  |
| 316 | 151        | 162      | TKLTEEEKNRLN     | none         | 3 (2)   | 492.265 | 17.03                | 3.2   | 50.5   | x               | x                 | x               | 1  |
| 317 | 151        | 163      | TKLTEEEKNRLNF    | none         | 3       | 541.289 | 29.00                | 3.5   | 67.3   | x               | x                 | x               | 1  |
| 318 | 151        | 164      | TKLTEEEKNRLNFL   | none         | 2 (3)   | 867.971 | 36.78                | 4.1   | 90.9   | x               | x                 | x               | 1  |
| 319 | 151        | 165      | TKLTEEEKNRLNFLK  | none         | 2 (3,4) | 932.020 | 31.80                | 4.7   | 87.9   | x               | x                 | x               | 1; 5   |
| 320 | 152        | 163      | KLTEEEKNRLNF     | none         | 3       | 507.605 | 26.59                | 3.1   | 28.4   | x               | x                 | x               | 1; 5   |
| 321 | 152        | 164      | KLTEEEKNRLNFL    | none         | 3 (2)   | 545.301 | 35.24                | 3.7   | 78.6   | x               | x                 | x               | 5  |
| 322 | 152        | 165      | KLTEEEKNRLNFLK   | none         | 4 (3)   | 441.250 | 29.77                | 2.8   | 31.8   | x               | x                 |                 | 5  |
| 323 | 153        | 161      | LTEEEKNRL        | none         | 2       | 566.302 | 16.94                | 1.9   | 39.3   | x               | x                 | x               | 1; 5   |
| 324 | 153        | 164      | LTEEEKNRLNFL     | none         | 2 (3)   | 753.403 | 38.44                | 3.5   | 74.6   | x               | x                 | x               | 1  |
| 325 | 153        | 165      | LTEEEKNRLNFLK    | none         | 3 (2)   | 545.301 | 32.01                | 3.4   | 44.1   | x               | x                 | x               | 1  |
| 326 | 154        | 163      | TEEEKNRLNF       | none         | 2 (3)   | 640.317 | 24.36                | 3.0   | 56.3   | x               | x                 | x               | 1  |
| 327 | 154        | 164      | TEEEKNRLNFL      | none         | 2 (3)   | 696.860 | 35.53                | 3.8   | 69.5   | x               | x                 | x               | 5  |
| 328 | 154        | 165      | TEEEKNRLNFLK     | none         | 3       | 507.604 | 27.91                | 3.1   | 40.3   | x               | x                 | x               | 5  |
| 329 | 155        | 164      | EEEKNRLNFL       | none         | 2       | 646.336 | 35.55                | 2.2   | 56.7   | x               | x                 | x               | 1  |
| 330 | 162        | 169      | NFLKKISQ         | none         | 2       | 489.291 | 24.74                | 2.4   | 44.6   |                 |                   | x               |  |
| 331 | 170        | 179      | RYQKFALPQY       | none         | 2 (3)   | 657.354 | 35.84                | 2.1   | 55.8   |                 |                   | x               |  |
| 332 | 171        | 179      | YQKFALPQY        | none         | 2       | 579.304 | 40.61                | 2.2   | 56.2   |                 |                   | x               |  |
| 333 | 171        | 180      | YQKFALPQYL       | none         | 2       | 635.847 | 50.00                | 2.2   | 49.6   | x               | x                 | x               | 1; 5   |
| 334 | 172        | 179      | QKFALPQY         | none         | 2       | 497.771 | 37.54                | 1.5   | 43.3   |                 |                   | x               |  |
| 335 | 172        | 180      | QKFALPQYL        | none         | 2       | 554.313 | 47.59                | 1.8   | 38.7   | x               | x                 | x               | 5  |
| 336 | 174        | 181      | FALPQYLYK        | none         | 2       | 490.284 | 44.25                | 2.3   | 38.6   | x               | x                 | x               | 1  |
| 337 | 174        | 187      | FALPQYLKTVYQHQ   | none         | 3 (2)   | 579.310 | 48.81                | 3.7   | 66.7   | x               | x                 |                 | 1  |
| 338 | 175        | 188      | ALPQYLKTVYQHQK   | none         | 3       | 572.985 | 34.66                | 2.8   | 40.6   | x               | x                 |                 | 5  |
| 339 | 176        | 183      | LPQYLKTV         | none         | 2       | 481.288 | 35.91                | 2.7   | 43.1   | x               | x                 |                 | 1  |
| 340 | 176        | 185      | LPQYLKTVYQ       | none         | 2       | 626.849 | 38.96                | 2.4   | 62.6   | x               | x                 | x               |  |
| 341 | 189        | 196      | AMKPWIQP         | none         | 2       | 485.761 | 36.69                | 2.4   | 38.2   | x               | x                 | x               | 1  |
| 342 | 189        | 196      | AmKPWIQP         | M2(Ox)       | 2       | 493.759 | 30.92                | 2.0   | 30.9   | x               | x                 |                 | 1  |

| Nr.  | Start pos. | End pos. | Sequence         | Modification | z     | m/z     | t <sub>r</sub> (min) | Xcorr | -10lgP | RM <sup>a</sup> | UH T <sup>a</sup> | IF <sup>a</sup> | Literature (milk <sup>1-6</sup> , colostrum <sup>7</sup> ) |
|--|------------|----------|------------------|--------------|-------|---------|----------------------|-------|--------|-----------------|-------------------|-----------------|--|
| 343  | 189        | 197      | AMKPWIQPK        | none         | 2     | 549.808 | 27.15                | 2.2   | 43.6   |                 | x                 | x               | 5  |
| 344  | 189        | 198      | AMKPWIQPKT       | none         | 3 (2) | 400.557 | 28.88                | 3.1   | 45.9   | x               | x                 | x               | 1  |
| 345  | 189        | 198      | AmKPWIQPKT       | M2(Ox)       | 3 (2) | 405.889 | 23.78                | 2.6   | 35.3   | x               | x                 |                 | 1  |
| 346  | 189        | 203      | AMKPWIQPKTKVIPY  | none         | 4 (3) | 450.761 | 39.31                | 2.5   | 29.0   |                 |                   | x               |  |
| 347  | 191        | 198      | KPWIQPKT         | none         | 2     | 499.294 | 21.54                | 2.1   | 41.7   | x               | x                 |                 |  |
| 348  | 198        | 204      | TKVIPYV          | none         | 2     | 410.252 | 34.16                | 1.9   | 36.6   | x               | x                 | x               | 1  |
| 349  | 198        | 205      | TKVIPYVR         | none         | 2     | 488.301 | 24.73                | 2.5   | 37.9   | x               | x                 | x               | 1  |
| 350  | 198        | 206      | TKVIPYVRY        | none         | 2     | 569.833 | 32.02                | 2.4   | 46.1   | x               | x                 | x               | 1; 5   |
| 351  | 198        | 207      | TKVIPYVRYL       | none         | 3 (2) | 417.919 | 41.48                | 2.9   | 52.3   | x               | x                 | x               | 1; 3; 4; 5   |
| 352  | 199        | 205      | KVIPYVR          | none         | 2     | 437.778 | 22.91                | 2.2   | 21.9   | x               | x                 |                 |  |
| 353  | 199        | 206      | KVIPYVRY         | none         | 2     | 519.310 | 30.12                | 1.9   | 23.4   | x               | x                 |                 |  |
| 354  | 199        | 207      | KVIPYVRYL        | none         | 2     | 575.852 | 39.86                | 2.4   | 39.9   | x               | x                 | x               | 3;   |
| 355  | 200        | 206      | VIPYVRY          | none         | 2     | 455.263 | 35.45                | 1.5   | 29.7   | x               | x                 | x               |  |
| 356  | 200        | 207      | VIPYVRYL         | none         | 2     | 511.804 | 46.76                | 1.6   | 40.6   | x               | x                 | x               | 1; 3; 5  |
| 357  | 201        | 207      | IPYVRYL          | none         | 2     | 462.271 | 42.31                | 1.8   | 41.4   | x               | x                 | x               | 1; 4   |
| <b>Apolipoprotein A-I (P15497)</b>               |            |          |                  |              |       |         |                      |       |        |                 |                   |                 |  |
| 358  | 235        | 247      | AAIDEASKKLNAQ    | none         | 2     | 679.868 | 22.31                | 3.6   | 74.7   |                 |                   | x               |  |
| <b>Beta-1,4-galactosyltransferase 1 (P08037)</b> |            |          |                  |              |       |         |                      |       |        |                 |                   |                 |  |
| 359  | 69         | 79       | AIGQPSGELRL      | none         | 2     | 570.822 | 37.19                | 2.2   | 37.5   |                 |                   | x               |  |
| 360  | 54         | 69       | VGVHPPLQGSSHGAAA | none         | 3     | 495.590 | 22.64                | 2.8   | 31.5   | x               | x                 |                 |  |
| <b>Beta-2-microglobulin (P01888)</b>             |            |          |                  |              |       |         |                      |       |        |                 |                   |                 |  |
| 361  | 1          | 10       | IQRPPKIQVY       | none         | 2     | 621.371 | 29.68                | 2.1   | 49.7   |                 |                   | x               |  |
| <b>Beta-casein (P02666)</b>                      |            |          |                  |              |       |         |                      |       |        |                 |                   |                 |  |
| 362  | 1          | 7        | RELEELN          | none         | 2     | 451.731 | 20.15                | 1.7   | 30.3   |                 | x                 |                 |  |
| 363  | 1          | 10       | RELEELNVPG       | none         | 2     | 578.302 | 33.29                | 1.7   | 43.5   | x               | x                 | x               |  |
| 364  | 1          | 11       | RELEELNVPGE      | none         | 2     | 642.824 | 34.48                | 2.5   | 54.6   | x               | x                 | x               | 1; 4; 6  |
| 365  | 1          | 14       | RELEELNVPGEIVE   | none         | 2     | 813.425 | 43.62                | 2.4   | 69.3   |                 | x                 | x               | 5  |
| 366  | 1          | 15       | RELEELNVPGEIVES  | none         | 2     | 856.939 | 43.36                | 2.6   | 70.3   | x               | x                 | x               | 1; 5   |
| 367  | 1          | 16       | RELEELNVPGEIVESL | none         | 2     | 913.483 | 58.41                | 2.5   | 55.3   | x               | x                 | x               |  |

| Nr. | Start pos. | End pos. | Sequence                     | Modification | z       | m/z      | t <sub>r</sub> (min) | Xcorr | -10lgP | RM <sup>a</sup> | UH T <sup>a</sup> | IF <sup>a</sup> | Literature (milk <sup>1-6</sup> , colostrum <sup>7</sup> ) |
|-----|------------|----------|------------------------------|--------------|---------|----------|----------------------|-------|--------|-----------------|-------------------|-----------------|--|
| 368 | 1          | 16       | RELEELNVPGEIVEsL             | S15(Phospho) | 2       | 953.466  | 54.67                | 3.5   | 57.2   |                 | x                 | x               | 3  |
| 369 | 1          | 22       | RELEELNVPGEIVESLSSSEES       | none         | 2       | 1216.588 | 58.86                | 4.3   | 82.0   | x               | x                 | x               | 1; 5   |
| 370 | 1          | 25       | RELEELNVPGEIVESLSSSEESITR    | none         | 3       | 934.805  | 61.58                | 5.3   | 76.1   | x               | x                 | x               | 1; 2; 3; 5   |
| 371 | 1          | 27       | RELEELNVPGEIVESLSSSEESITRIN  | none         | 3       | 1010.515 | 64.91                | 4.4   | 49.8   | x               | x                 | x               | 1; 3; 5  |
| 372 | 1          | 27       | RELEELNVPGEIVESLSSSEESITRIN  | S19(Phospho) | 3       | 1037.170 | 59.61                | 4.7   | 66.5   | x               | x                 | x               | 5  |
| 373 | 1          | 27       | RELEELNVPGEIVESLSSsSEESITRIN | S18(Phospho) | 3       | 1037.173 | 62.51                | 4.7   | 71.9   | x               | x                 | x               | 5  |
| 374 | 1          | 28       | RELEELNVPGEIVESLSSSEESITRINK | none         | 3 (4)   | 1053.213 | 62.25                | 7.5   | 108.7  | x               | x                 | x               | 5  |
| 375 | 1          | 28       | RELEELNVPGEIVESLSSsEESITRINK | S19(Phospho) | 4       | 810.153  | 56.41                | 3.0   | 61.1   | x               | x                 | x               | 5  |
| 376 | 1          | 28       | RELEELNVPGEIVESLsSSEESITRINK | S17(Phospho) | 4       | 810.156  | 56.89                | 6.0   | 83.9   | x               | x                 | x               | 5  |
| 377 | 1          | 28       | RELEELNVPGEIVESLsSSEESITRINK | S18(Phospho) | 3 (4)   | 1079.871 | 60.17                | 6.3   | 23.6   | x               | x                 | x               | 5  |
| 378 | 2          | 11       | ELEELNVPGE                   | none         | 2       | 564.775  | 39.27                | 2.1   | 44.9   | x               | x                 | x               | 5; 7   |
| 379 | 2          | 15       | ELEELNVPGEIVES               | none         | 2       | 778.888  | 48.81                | 2.5   | 52.2   | x               | x                 | x               | 5  |
| 380 | 7          | 16       | NVPGEIVESL                   | none         | 2       | 528.782  | 47.86                | 2.1   | 56.8   |                 |                   | x               |  |
| 381 | 16         | 25       | LSSsEESITR                   | S4(Phospho)  | 2       | 594.760  | 21.90                | 2.3   | 29.1   | x               | x                 | x               |  |
| 382 | 17         | 27       | SSSEESITRIN                  | none         | 2       | 611.797  | 22.75                | 1.8   | 45.8   |                 |                   | x               |  |
| 383 | 18         | 27       | SSEESITRIN                   | none         | 2       | 568.283  | 22.23                | 2.6   | 48.4   |                 |                   | x               |  |
| 384 | 26         | 48       | INKKIEKFQSEEQQQTEDELQDK      | none         | 4       | 709.605  | 29.21                | 4.1   | 24.2   | x               | x                 | x               |  |
| 385 | 26         | 48       | INKKIEKFQsEEQQQTEDELQDK      | S10(Phospho) | 3 (4)   | 972.461  | 30.94                | 5.4   | 54.7   | x               | x                 | x               |  |
| 386 | 29         | 39       | KIEKFQsEEQQ                  | S7(Phospho)  | 2       | 737.334  | 17.73                | 3.1   | 45.3   | x               | x                 | x               |  |
| 387 | 29         | 40       | KIEKFQsEEQQQ                 | S7(Phospho)  | 2       | 801.364  | 18.30                | 3.7   | 47.9   | x               | x                 | x               |  |
| 388 | 29         | 42       | KIEKFQsEEQQQTE               | S7(Phospho)  | 2       | 916.410  | 20.81                | 3.3   | 43.6   | x               | x                 | x               |  |
| 389 | 29         | 43       | KIEKFQsEEQQQTED              | S7(Phospho)  | 2 (3)   | 973.922  | 21.13                | 3.9   | 53.5   | x               | x                 | x               |  |
| 390 | 29         | 46       | KIEKFQsEEQQQTEDELQ           | S7(Phospho)  | 3 (2)   | 773.011  | 30.02                | 4.6   | 38.4   | x               | x                 | x               |  |
| 391 | 29         | 47       | KIEKFQSEEQQQTEDELQD          | none         | 3 (2)   | 784.699  | 27.70                | 5.0   | 67.4   | x               | x                 | x               |  |
| 392 | 29         | 47       | KIEKFQsEEQQQTEDELQD          | S7(Phospho)  | 3 (2)   | 811.356  | 30.43                | 5.8   | 67.3   | x               | x                 | x               |  |
| 393 | 29         | 48       | KIEKFQSEEQQQTEDELQDK         | none         | 3 (2,4) | 827.398  | 26.72                | 7.9   | 98.6   | x               | x                 | x               | 1; 3; 5  |
| 394 | 29         | 48       | KIEKFQsEEQQQTEDELQDK         | S7(Phospho)  | 3 (2,4) | 854.054  | 29.03                | 7.9   | 85.7   | x               | x                 | x               | 1; 3; 5  |
| 395 | 29         | 52       | KIEKFQSEEQQQTEDELQDKIHPF     | none         | 4       | 744.365  | 40.63                | 5.4   | 57.0   | x               | x                 | x               | 5  |
| 396 | 29         | 52       | KIEKFQsEEQQQTEDELQDKIHPF     | S7(Phospho)  | 4 (3)   | 764.357  | 42.50                | 5.8   | 46.8   | x               | x                 | x               |  |

| Nr. | Start pos. | End pos. | Sequence                      | Modification | z       | m/z      | t <sub>r</sub> (min) | Xcorr | -10lgP | RM <sup>a</sup> | UH T <sup>a</sup> | IF <sup>a</sup> | Literature (milk <sup>1-6</sup> , colostrum <sup>7</sup> ) |
|-----|------------|----------|-------------------------------|--------------|---------|----------|----------------------|-------|--------|-----------------|-------------------|-----------------|--|
| 397 | 29         | 53       | KIEKFQSEEQQQTEDELQDKIHPFA     | none         | 4       | 762.125  | 40.51                | 6.2   | 65.4   | x               | x                 | x               | 2  |
| 398 | 29         | 53       | KIEKFQsEEQQQTEDELQDKIHPFA     | S7(Phospho)  | 4 (3)   | 782.117  | 42.22                | 5.4   | 54.7   | x               | x                 | x               |  |
| 399 | 29         | 55       | KIEKFQsEEQQQTEDELQDKIHPFAQT   | S7(Phospho)  | 4 (3)   | 839.395  | 41.94                | 6.8   | 40.4   | x               | x                 | x               |  |
| 400 | 29         | 56       | KIEKFQSEEQQQTEDELQDKIHPFAQTQ  | none         | 4       | 851.417  | 39.67                | 6.0   | 43.3   | x               | x                 | x               |  |
| 401 | 29         | 56       | KIEKFQSEEQQQTEDELQDKIHPFAQTQ  | S7(Phospho)  | 4 (3)   | 871.409  | 41.33                | 6.6   | 43.8   | x               | x                 | x               |  |
| 402 | 29         | 57       | KIEKFQSEEQQQTEDELQDKIHPFAQTQS | none         | 3 (4,5) | 1163.900 | 39.49                | 6.0   | 78.7   | x               | x                 | x               |  |
| 403 | 29         | 57       | KIEKFQsEEQQQTEDELQDKIHPFAQTQS | S7(Phospho)  | 4 (3)   | 893.167  | 41.22                | 6.0   | 48.4   | x               | x                 | x               |  |
| 404 | 30         | 39       | IEKFQsEEQQ                    | S6(Phospho)  | 2       | 673.287  | 20.70                | 3.1   | 39.2   | x               | x                 | x               |  |
| 405 | 30         | 40       | IEKFQsEEQQQ                   | S6(Phospho)  | 2       | 737.317  | 21.03                | 3.7   | 53.8   |                 |                   | x               |  |
| 406 | 30         | 43       | IEKFQsEEQQQTED                | S6(Phospho)  | 2       | 909.874  | 23.92                | 3.4   | 45.0   |                 | x                 | x               | 7  |
| 407 | 30         | 47       | IEKFQSEEQQQTEDELQD            | none         | 2       | 1112.498 | 30.61                | 4.8   | 64.7   | x               | x                 | x               |  |
| 408 | 30         | 47       | IEKFQsEEQQQTEDELQD            | S6(Phospho)  | 2       | 1152.483 | 33.60                | 6.4   | 74.1   | x               | x                 | x               |  |
| 409 | 30         | 48       | IEKFQSEEQQQTEDELQDK           | none         | 3 (2)   | 784.701  | 28.96                | 7.4   | 82.0   | x               | x                 | x               | 3; 5   |
| 410 | 30         | 48       | IEKFQsEEQQQTEDELQDK           | S6(Phospho)  | 3 (2)   | 811.356  | 31.54                | 7.0   | 71.9   | x               | x                 | x               | 3; 5   |
| 411 | 30         | 53       | IEKFQsEEQQQTEDELQDKIHPFA      | S6(Phospho)  | 3       | 999.791  | 44.74                | 5.9   | 56.4   | x               | x                 | x               |  |
| 412 | 30         | 56       | IEKFQsEEQQQTEDELQDKIHPFAQTQ   | S6(Phospho)  | 3       | 1118.845 | 43.65                | 6.1   | 56.4   | x               | x                 | x               |  |
| 413 | 30         | 57       | IEKFQsEEQQQTEDELQDKIHPFAQTQS  | S6(Phospho)  | 3       | 1147.857 | 43.52                | 6.2   | 43.8   | x               | x                 | x               |  |
| 414 | 32         | 48       | KFQSEEQQQTEDELQDK             | none         | 3 (2)   | 703.989  | 24.49                | 5.6   | 61.2   | x               | x                 | x               | 1; 3; 5  |
| 415 | 32         | 48       | KFQsEEQQQTEDELQDK             | S4(Phospho)  | 2 (3)   | 1095.465 | 28.30                | 6.8   | 77.9   | x               | x                 | x               | 3; 5   |
| 416 | 33         | 48       | FQSEEQQQTEDELQDK              | none         | 2 (3)   | 991.432  | 26.81                | 5.6   | 100.3  | x               | x                 | x               | 3; 5   |
| 417 | 33         | 48       | FQsEEQQQTEDELQDK              | S3(Phospho)  | 2 (3)   | 1031.416 | 30.17                | 7.1   | 92.6   | x               | x                 | x               | 3; 5   |
| 418 | 33         | 51       | FQSEEQQQTEDELQDKIHP           | none         | 3       | 777.024  | 35.99                | 3.2   | 35.8   | x               | x                 | x               |  |
| 419 | 33         | 53       | FQsEEQQQTEDELQDKIHPFA         | S3(Phospho)  | 3       | 876.382  | 45.96                | 4.7   | 59.7   | x               | x                 | x               |  |
| 420 | 33         | 56       | FQSEEQQQTEDELQDKIHPFAQTQ      | none         | 3       | 968.781  | 41.90                | 3.8   | 55.2   | x               | x                 |                 |  |
| 421 | 33         | 57       | FQSEEQQQTEDELQDKIHPFAQTQS     | none         | 3       | 997.794  | 41.74                | 4.6   | 57.4   | x               | x                 | x               |  |
| 422 | 33         | 57       | FQsEEQQQTEDELQDKIHPFAQTQS     | S3(Phospho)  | 3       | 1024.448 | 44.37                | 4.2   | 56.3   | x               | x                 | x               |  |
| 423 | 35         | 48       | SEEQQQTEDELQDK                | none         | 2       | 853.870  | 20.82                | 4.8   | 98.9   | x               | x                 | x               | 3; 5   |
| 424 | 35         | 48       | sEEQQQTEDELQDK                | S1(Phospho)  | 2       | 893.854  | 23.02                | 5.3   | 66.0   | x               | x                 | x               | 5  |
| 425 | 36         | 48       | EEQQQTEDELQDK                 | none         | 2       | 810.352  | 18.76                | 3.2   | 72.5   | x               | x                 | x               |  |

| Nr. | Start pos. | End pos. | Sequence                              | Modification | z       | m/z      | t <sub>r</sub> (min) | Xcorr | -10lgP | RM <sup>a</sup> | UH T <sup>a</sup> | IF <sup>a</sup> | Literature (milk <sup>1-6</sup> , colostrum <sup>7</sup> ) |
|-----|------------|----------|---------------------------------------|--------------|---------|----------|----------------------|-------|--------|-----------------|-------------------|-----------------|--|
| 426 | 37         | 48       | EQQQTEDELQDK                          | none         | 2       | 745.834  | 16.48                | 2.1   | 37.3   |                 | x                 | x               |  |
| 427 | 41         | 49       | TEDELQDKI                             | none         | 2       | 545.765  | 28.47                | 3.2   | 52.6   | x               | x                 |                 | 3; 5   |
| 428 | 43         | 51       | DELQDKIHP                             | none         | 2       | 547.777  | 25.81                | 2.2   | 37.7   | x               | x                 |                 |  |
| 429 | 49         | 56       | IHPFAQTQ                              | none         | 2       | 471.244  | 21.27                | 2.0   | 39.8   |                 | x                 |                 | 1  |
| 430 | 49         | 57       | IHPFAQTQS                             | none         | 2       | 514.761  | 21.63                | 2.0   | 52.0   |                 | x                 |                 |  |
| 431 | 57         | 68       | SLVYPFPGPPIP                          | none         | 2       | 650.852  | 55.36                | 2.1   | 54.5   |                 | x                 |                 | 5; 7   |
| 432 | 57         | 72       | SLVYPFPGPPIPNSLPQ                     | none         | 2       | 863.465  | 59.58                | 2.2   | 62.8   |                 | x                 |                 |  |
| 433 | 58         | 72       | LVYPFPGPPIPNSLPQ                      | none         | 2       | 819.948  | 58.52                | 2.4   | 62.8   |                 | x                 |                 |  |
| 434 | 69         | 91       | SLPQNIPPLTQTPVVVPPFLQPE               | none         | 2 (3)   | 1256.203 | 67.12                | 2.7   | 60.7   |                 | x                 |                 |  |
| 435 | 69         | 105      | SLPQNIPPLTQTPVVVPPFLQPEVMGVSKVKEAMAPK | none         | 4       | 992.555  | 65.99                | 2.0   | 22.5   | x               | x                 | x               |  |
| 436 | 73         | 91       | NIPPLTQTPVVVPPFLQPE                   | none         | 3 (2)   | 696.058  | 65.52                | 3.1   | 58.1   |                 | x                 |                 |  |
| 437 | 83         | 95       | VVPPFLQPEVmGV                         | M11(Ox)      | 2       | 714.384  | 55.39                | 1.6   | 33.8   | x               | x                 |                 | 5  |
| 438 | 83         | 98       | VVPPFLQPEVMGVSKV                      | none         | 2       | 863.484  | 56.12                | 1.9   | 57.3   | x               | x                 | x               | 5  |
| 439 | 84         | 95       | VPPFLQPEVMGV                          | none         | 2       | 656.852  | 59.21                | 1.9   | 43.6   | x               | x                 | x               | 1; 3; 5; 7   |
| 440 | 84         | 95       | VPPFLQPEVmGV                          | M10(Ox)      | 2       | 664.849  | 51.70                | 2.2   | 48.6   | x               | x                 | x               | 1; 5   |
| 441 | 84         | 98       | VPPFLQPEVMGVSKV                       | none         | 2       | 813.949  | 52.95                | 3.3   | 83.5   | x               | x                 | x               | 5  |
| 442 | 106        | 123      | HKEMPFPKYPVEPFTESEQ                   | none         | 3       | 731.024  | 41.93                | 3.6   | 50.7   | x               | x                 | x               | 2; 5   |
| 443 | 106        | 124      | HKEMPFPKYPVEPFTESEQS                  | none         | 3       | 760.033  | 41.43                | 3.7   | 59.6   | x               | x                 | x               | 1; 5   |
| 444 | 106        | 124      | HKEmPFPKYPVEPFTESEQS                  | M4(Ox)       | 3       | 765.364  | 37.95                | 3.6   | 42.2   | x               | x                 | x               | 5  |
| 445 | 106        | 125      | HKEMPFPKYPVEPFTESQL                   | none         | 3 (4,2) | 797.727  | 46.12                | 4.2   | 77.8   | x               | x                 | x               | 1; 2; 3; 5   |
| 446 | 106        | 125      | HKEmPFPKYPVEPFTESQL                   | M4(Ox)       | 3       | 803.061  | 43.36                | 3.4   | 46.5   | x               | x                 | x               | 5  |
| 447 | 106        | 132      | HKEMPFPKYPVEPFTESQLTLTDVEN            | none         | 3       | 1055.181 | 50.91                | 3.9   | 49.4   | x               | x                 | x               |  |
| 448 | 106        | 133      | HKEMPFPKYPVEPFTESQLTLTDVENL           | none         | 3 (4)   | 1092.878 | 57.53                | 4.3   | 37.4   | x               | x                 | x               | 5  |
| 449 | 107        | 124      | KEMPFPKYPVEPFTEQS                     | none         | 3       | 714.347  | 44.61                | 3.4   | 39.8   | x               | x                 |                 |  |
| 450 | 107        | 125      | KEMPFPKYPVEPFTESQL                    | none         | 3 (2)   | 752.040  | 49.39                | 4.1   | 66.8   | x               | x                 | x               | 5  |
| 451 | 107        | 125      | KEmPFPKYPVEPFTESQL                    | M3(Ox)       | 3       | 757.373  | 46.60                | 3.7   | 38.3   | x               | x                 |                 |  |
| 452 | 108        | 119      | EMPFPKYPVEPF                          | none         | 2       | 740.864  | 53.51                | 2.9   | 44.8   |                 | x                 |                 | 7  |
| 453 | 108        | 122      | EMPFPKYPVEPFTE                        | none         | 2       | 899.424  | 51.40                | 2.4   | 48.9   | x               | x                 | x               | 7  |
| 454 | 108        | 123      | EMPFPKYPVEFTESQ                       | none         | 2       | 963.454  | 50.75                | 3.8   | 70.5   | x               | x                 | x               | 7  |

| Nr. | Start pos. | End pos. | Sequence             | Modification | z     | m/z      | t <sub>r</sub> (min) | Xcorr | -10lgP | RM <sup>a</sup> | UH T <sup>a</sup> | IF <sup>a</sup> | Literature (milk <sup>1-6</sup> , colostrum <sup>7</sup> ) |
|-----|------------|----------|----------------------|--------------|-------|----------|----------------------|-------|--------|-----------------|-------------------|-----------------|--|
| 455 | 108        | 124      | EMPFPKYPVEPFTEQS     | none         | 2 (3) | 1006.970 | 50.30                | 4.2   | 89.8   | x               | x                 | x               | 1; 5; 7  |
| 456 | 108        | 124      | EmPFPKYPVEPFTEQS     | M2(Ox)       | 2     | 1014.968 | 45.27                | 3.9   | 78.9   | x               | x                 | x               | 7; 5   |
| 457 | 108        | 125      | EmPFPKYPVEPFTESQL    | M2(Ox)       | 2     | 1071.509 | 50.77                | 4.8   | 84.8   | x               | x                 | x               | 1; 5   |
| 458 | 108        | 126      | EMPFPKYPVEPFTESQLT   | none         | 2     | 1114.036 | 53.94                | 3.4   | 56.0   | x               | x                 |                 |  |
| 459 | 109        | 119      | MPFPKYPVEPF          | none         | 2     | 676.342  | 52.07                | 3.1   | 51.9   | x               |                   | x               | 7; 5   |
| 460 | 109        | 120      | MPFPKYPVEPFT         | none         | 2     | 726.864  | 50.70                | 3.4   | 63.0   | x               | x                 | x               | 7  |
| 461 | 109        | 123      | MPFPKYPVEPFTESQ      | none         | 2     | 898.932  | 49.28                | 4.3   | 77.2   | x               | x                 | x               | 7  |
| 462 | 109        | 124      | MPFPKYPVEPFTESQS     | none         | 2     | 942.447  | 48.83                | 4.3   | 92.9   | x               | x                 | x               | 1; 5   |
| 463 | 109        | 124      | mPFPKYPVEPFTESQS     | M1(Ox)       | 2     | 950.446  | 44.33                | 3.7   | 79.9   | x               | x                 |                 |  |
| 464 | 109        | 125      | MPFPKYPVEPFTESQL     | none         | 2     | 998.991  | 53.76                | 4.8   | 81.9   | x               | x                 | x               | 1; 5   |
| 465 | 109        | 125      | mPFPKYPVEPFTESQL     | M1(Ox)       | 2 (3) | 1006.988 | 49.86                | 4.4   | 76.1   | x               | x                 | x               |  |
| 466 | 109        | 126      | MPFPKYPVEPFTESQLT    | none         | 2     | 1049.514 | 52.68                | 3.8   | 53.4   | x               | x                 |                 |  |
| 467 | 111        | 124      | FPKYPVEPFTESQS       | none         | 2     | 828.402  | 42.85                | 3.5   | 65.3   | x               | x                 | x               |  |
| 468 | 111        | 125      | FPKYPVEPFTESQL       | none         | 2     | 884.943  | 48.88                | 4.5   | 97.3   | x               | x                 | x               | 1; 5; 7  |
| 469 | 114        | 125      | YPVEPFTESQL          | none         | 2     | 698.835  | 46.59                | 2.3   | 49.7   | x               | x                 | x               | 1; 5; 7  |
| 470 | 115        | 123      | PVEPFTESQ            | none         | 2     | 517.245  | 30.39                | 1.9   | 48.8   |                 |                   | x               | 7  |
| 471 | 115        | 124      | PVEPFTESQS           | none         | 2     | 560.762  | 30.03                | 2.3   | 45.6   |                 |                   | x               | 7  |
| 472 | 115        | 125      | PVEPFTESQL           | none         | 2     | 617.305  | 41.63                | 2.1   | 56.8   |                 |                   | x               | 7  |
| 473 | 124        | 133      | SLTLTDVENL           | none         | 2     | 552.793  | 51.64                | 2.4   | 62.9   |                 |                   | x               | 5  |
| 474 | 126        | 143      | TLTDVENLHLPLPLLQSW   | none         | 2 (3) | 1045.073 | 73.46                | 3.2   | 58.7   |                 |                   | x               |  |
| 475 | 128        | 143      | TDVENLHLPLPLLQSW     | none         | 2     | 938.005  | 70.48                | 3.6   | 57.9   |                 |                   | x               |  |
| 476 | 129        | 139      | DVENLHLPLPL          | none         | 2     | 630.354  | 59.63                | 2.3   | 34.8   |                 |                   | x               |  |
| 477 | 129        | 143      | DVENLHLPLPLLQSW      | none         | 2     | 887.482  | 72.06                | 3.2   | 57.8   |                 |                   | x               |  |
| 478 | 132        | 143      | NLHLPLPLLQSW         | none         | 2     | 715.912  | 68.77                | 2.5   | 52.1   |                 |                   | x               |  |
| 479 | 134        | 143      | HLPLPLLQSW           | none         | 2     | 602.349  | 61.21                | 2.6   | 46.2   |                 |                   | x               |  |
| 480 | 144        | 154      | MHQPHQPLPPT          | none         | 2     | 641.821  | 20.36                | 2.5   | 52.3   |                 |                   | x               |  |
| 481 | 144        | 162      | MHQPHQPLPPTVMFPPQSV  | none         | 3     | 723.365  | 45.71                | 3.4   | 45.7   |                 |                   | x               | 7  |
| 482 | 144        | 162      | mHQPHQPLPPTVMFPPQSV  | M1(Ox)       | 3     | 728.696  | 44.15                | 2.6   | 28.9   |                 |                   | x               |  |
| 483 | 144        | 163      | MHQPHQPLPPTVMFPPQSVL | none         | 3     | 761.061  | 51.23                | 2.8   | 46.5   |                 |                   | x               | 7  |

| Nr. | Start pos. | End pos. | Sequence                      | Modification | z     | m/z      | t <sub>r</sub> (min) | Xcorr | -10lgP | RM <sup>a</sup> | UH T <sup>a</sup> | IF <sup>a</sup> | Literature (milk <sup>1-6</sup> , colostrum <sup>7</sup> ) |
|-----|------------|----------|-------------------------------|--------------|-------|----------|----------------------|-------|--------|-----------------|-------------------|-----------------|--|
| 484 | 144        | 165      | MHQPHQPLPPTVMFPPQSVL          | none         | 3     | 827.764  | 57.91                | 3.5   | 45.2   |                 |                   | x               |  |
| 485 | 144        | 165      | mHQPHQPLPPTVMFPPQSVL          | M1(Ox)       | 3     | 833.097  | 57.74                | 2.7   | 20.5   |                 |                   | x               |  |
| 486 | 144        | 168      | MHQPHQPLPPTVMFPPQSVL          |              | 3     | 928.475  | 54.60                | 2.9   | 38.3   |                 |                   | x               |  |
| 487 | 161        | 169      | SVLSLSQSK                     | none         | 2     | 474.770  | 26.09                | 2.3   | 53.0   |                 |                   | x               |  |
| 488 | 163        | 175      | LSLSQSKVLPVPQ                 | none         | 2     | 698.414  | 40.81                | 3.0   | 51.2   |                 |                   | x               |  |
| 489 | 163        | 182      | LSLSQSKVLPVPQKAVPYQP          | none         | 3     | 727.089  | 42.38                | 3.7   | 48.2   |                 |                   | x               |  |
| 490 | 163        | 190      | LSLSQSKVLPVPQKAVPYQPQRDMPIQAF | none         | 3 (4) | 1046.580 | 50.43                | 5.0   | 73.9   | x               | x                 | x               |  |
| 491 | 164        | 175      | SLSQSKVLPVPQ                  | none         | 2     | 641.872  | 33.16                | 2.6   | 63.0   | x               |                   | x               |  |
| 492 | 164        | 176      | SLSQSKVLPVPQK                 | none         | 2 (3) | 705.920  | 27.20                | 3.8   | 71.4   | x               | x                 | x               | 1  |
| 493 | 164        | 182      | SLSQSKVLPVPQKAVPYQP           | none         | 3 (2) | 689.394  | 37.37                | 3.7   | 79.8   |                 |                   | x               |  |
| 494 | 164        | 190      | SLSQSKVLPVPQKAVPYQPQRDMPIQAF  | none         | 3 (4) | 1008.884 | 47.49                | 5.0   | 70.9   | x               | x                 | x               | 5  |
| 495 | 165        | 175      | LSQSKVLPVPQ                   | none         | 2     | 598.358  | 31.14                | 2.5   | 35.7   | x               | x                 | x               |  |
| 496 | 166        | 175      | SQSKVLPVPQ                    | none         | 2     | 541.812  | 26.71                | 2.5   | 56.1   |                 |                   | x               |  |
| 497 | 166        | 176      | SQSKVLPVPQK                   | none         | 2 (3) | 605.860  | 20.63                | 3.3   | 68.0   | x               | x                 | x               |  |
| 498 | 166        | 182      | SQSKVLPVPQKAVPYQP             | none         | 2 (3) | 933.533  | 33.87                | 2.6   | 65.6   |                 |                   | x               |  |
| 499 | 166        | 190      | SQSKVLPVPQKAVPYQPQRDMPIQAF    | none         | 3     | 942.179  | 45.43                | 4.6   | 58.7   | x               |                   | x               |  |
| 500 | 167        | 175      | QSKVLPVPQ                     | none         | 2     | 498.297  | 26.45                | 1.7   | 23.7   |                 |                   | x               |  |
| 501 | 168        | 175      | SKVLPVPQ                      | none         | 2     | 434.267  | 26.11                | 2.3   | 30.6   |                 |                   | x               |  |
| 502 | 168        | 182      | SKVLPVPQKAVPYQP               | none         | 3     | 550.991  | 33.37                | 1.9   | 56.4   |                 |                   | x               |  |
| 503 | 170        | 182      | VLPVPQKAVPYQP                 | none         | 2     | 718.420  | 36.52                | 2.2   | 74.9   |                 |                   | x               |  |
| 504 | 170        | 189      | VLPVPQKAVPYQPQRDMPQA          | none         | 3     | 749.748  | 41.93                | 3.2   | 54.9   | x               | x                 | x               | 5  |
| 505 | 170        | 190      | VLPVPQKAVPYQPQRDMPIQAF        | none         | 3     | 798.771  | 48.74                | 3.6   | 66.4   | x               | x                 | x               | 5  |
| 506 | 170        | 190      | VLPVPQKAVPYPQRDmPIQAF         | M16(Ox)      | 3     | 804.105  | 44.20                | 3.3   | 67.4   | x               | x                 | x               |  |
| 507 | 171        | 179      | LPVPQKAVP                     | none         | 2     | 474.797  | 28.99                | 1.9   | 39.6   |                 |                   | x               |  |
| 508 | 171        | 182      | LPVPQKAVPYQP                  | none         | 2     | 668.884  | 33.86                | 1.9   | 57.1   |                 |                   | x               |  |
| 509 | 171        | 186      | LPVPQKAVPYPQRDMP              | none         | 3     | 612.665  | 36.41                | 3.3   | 61.9   | x               | x                 | x               | 5  |
| 510 | 171        | 189      | LPVPQKAVPYPQRDMPQA            | none         | 3     | 716.725  | 40.01                | 3.4   | 60.3   | x               | x                 | x               |  |
| 511 | 171        | 190      | LPVPQKAVPYPQRDMPIQAF          | none         | 3     | 765.748  | 47.14                | 2.5   | 24.2   | x               | x                 | x               | 5  |
| 512 | 176        | 182      | KAVPYQP                       | none         | 2     | 401.726  | 17.58                | 2.3   | 32.7   |                 |                   | x               |  |

| Nr. | Start pos. | End pos. | Sequence                          | Modification | z     | m/z      | t <sub>r</sub> (min) | Xcorr | -10lgP | RM <sup>a</sup> | UH T <sup>a</sup> | IF <sup>a</sup> | Literature (milk <sup>1-6</sup> , colostrum <sup>7</sup> ) |
|-----|------------|----------|-----------------------------------|--------------|-------|----------|----------------------|-------|--------|-----------------|-------------------|-----------------|--|
| 513 | 176        | 190      | KAVPYPQRDMPIQAF                   | none         | 2 (3) | 880.961  | 40.78                | 3.3   | 78.0   |                 | x                 | x               |  |
| 514 | 177        | 188      | AVPYPQRDMPIQ                      | none         | 2     | 707.863  | 34.03                | 2.3   | 53.9   | x               | x                 | x               | 7  |
| 515 | 177        | 189      | AVPYPQRDMPIQA                     | none         | 2     | 743.380  | 36.24                | 2.7   | 60.2   | x               | x                 | x               |  |
| 516 | 177        | 189      | AVPYPQRDmPIQA                     | M9(Ox)       | 2     | 751.378  | 29.73                | 2.2   | 50.8   | x               | x                 | x               |  |
| 517 | 177        | 190      | AVPYPQRDMPIQAF                    | none         | 2     | 816.914  | 46.08                | 2.3   | 69.2   |                 | x                 |                 | 5; 7   |
| 518 | 177        | 190      | AVPYPQRDmPIQAF                    | M9(Ox)       | 2     | 824.913  | 39.44                | 2.7   | 65.3   |                 | x                 |                 |  |
| 519 | 177        | 191      | AVPYPQRDMPIQ AFL                  | none         | 2     | 873.458  | 56.17                | 2.0   | 51.9   |                 | x                 |                 |  |
| 520 | 177        | 209      | AVPYPQRDMPIQ AFLLYQEPVLGPVRGPFIIV | none         | 3     | 1241.015 | 76.08                | 4.9   | 56.7   | x               | x                 | x               | 5  |
| 521 | 177        | 209      | AVPYPQRDmPIQ AFLLYQEPVLGPVRGPFIIV | M9(Ox)       | 3     | 1246.351 | 73.24                | 4.2   | 43.1   | x               | x                 | x               |  |
| 522 | 178        | 184      | VPYPQRD                           | none         | 2     | 437.723  | 16.09                | 1.4   | 32.5   | x               | x                 |                 |  |
| 523 | 178        | 186      | VPYPQRDmP                         | M8(Ox)       | 2     | 559.768  | 21.20                | 2.3   | 42.8   | x               | x                 |                 | 7  |
| 524 | 178        | 188      | VPYPQRDMPIQ                       | none         | 2     | 672.341  | 32.40                | 3.4   | 60.2   | x               | x                 | x               | 1; 7   |
| 525 | 178        | 188      | VPYPQRDmPIQ                       | M8(Ox)       | 2     | 680.338  | 25.25                | 2.9   | 47.6   | x               | x                 |                 | 1; 7   |
| 526 | 178        | 189      | VPYPQRDMPIQA                      | none         | 2     | 707.860  | 34.71                | 2.8   | 68.9   | x               | x                 | x               | 1; 4; 5  |
| 527 | 178        | 189      | VPYPQRDmPIQA                      | M8(Ox)       | 2     | 715.858  | 28.04                | 2.7   | 60.1   | x               | x                 | x               | 1  |
| 528 | 178        | 190      | VPYPQRDMPIQAF                     | none         | 2     | 781.395  | 45.14                | 3.2   | 76.2   | x               | x                 | x               |  |
| 529 | 178        | 191      | VPYPQRDMPIQ AFL                   | none         | 2     | 837.938  | 55.53                | 3.2   | 61.7   | x               | x                 |                 | 1; 2; 5  |
| 530 | 178        | 191      | VPYPQRDmPIQ AFL                   | M8(Ox)       | 2     | 845.934  | 48.70                | 2.6   | 35.7   | x               | x                 |                 |  |
| 531 | 180        | 189      | YPQRDmPIQA                        | M6(Ox)       | 2     | 617.797  | 22.13                | 2.0   | 38.9   | x               |                   |                 |  |
| 532 | 180        | 190      | YPQRDMPIQAF                       | none         | 2     | 683.336  | 41.11                | 2.4   | 43.1   |                 | x                 |                 |  |
| 533 | 183        | 190      | RDMPIQAF                          | none         | 2     | 489.247  | 36.95                | 1.7   | 40.9   |                 | x                 |                 |  |
| 534 | 183        | 190      | RDmPIQAF                          | M3(Ox)       | 2     | 497.245  | 29.32                | 2.0   | 36.6   |                 | x                 |                 |  |
| 535 | 191        | 198      | LLYQEPV L                         | none         | 2     | 487.781  | 47.22                | 1.6   | 33.2   |                 | x                 |                 |  |
| 536 | 191        | 201      | LLYQEPVLGPV                       | none         | 2     | 614.354  | 51.48                | 2.4   | 48.9   | x               | x                 |                 | 5  |
| 537 | 191        | 206      | LLYQEPVLGPVRGPFP                  | none         | 2 (3) | 891.506  | 55.05                | 4.2   | 89.3   |                 | x                 |                 | 6; 7   |
| 538 | 191        | 207      | LLYQEPVLGPVRGPFP I                | none         | 2 (3) | 948.046  | 61.12                | 3.5   | 78.7   | x               | x                 | x               |  |
| 539 | 191        | 208      | LLYQEPVLGPVRGPFP II               | none         | 2 (3) | 1004.586 | 65.35                | 4.0   | 80.7   | x               | x                 | x               | 2  |
| 540 | 191        | 209      | LLYQEPVLGPVRGPFP II V             | none         | 2 (3) | 1054.120 | 67.06                | 4.2   | 89.0   | x               | x                 | x               | 1; 5; 6  |
| 541 | 192        | 206      | LYQEPVLGPVRGPFP                   | none         | 2     | 834.960  | 50.72                | 4.0   | 84.4   |                 | x                 |                 | 2; 6   |

| Nr.                                | Start pos. | End pos. | Sequence           | Modification | z     | m/z     | t <sub>r</sub> (min) | Xcorr | -10lgP | RM <sup>a</sup> | UH T <sup>a</sup> | IF <sup>a</sup> | Literature (milk <sup>1-6</sup> , colostrum <sup>7</sup> ) |
|------------------------------------|------------|----------|--------------------|--------------|-------|---------|----------------------|-------|--------|-----------------|-------------------|-----------------|--|
| 542                                | 192        | 207      | LYQEPVLGPVRGPFPPI  | none         | 2     | 891.503 | 57.40                | 3.2   | 81.7   | x               | x                 | x               | 2  |
| 543                                | 192        | 208      | LYQEPVLGPVRGPFPPII | none         | 2     | 948.043 | 62.13                | 4.2   | 88.2   | x               | x                 | x               | 2; 5; 6  |
| 544                                | 192        | 209      | LYQEPVLGPVRGPFPPIV | none         | 2 (3) | 997.578 | 63.95                | 3.8   | 82.3   | x               | x                 | x               | 1; 4; 5; 6   |
| 545                                | 193        | 202      | YQEPVLGPVR         | none         | 2     | 579.318 | 32.25                | 2.7   | 57.7   | x               | x                 | x               | 1; 5; 7  |
| 546                                | 193        | 206      | YQEPVLGPVRGPFP     | none         | 2     | 778.417 | 48.25                | 3.1   | 87.7   |                 | x                 | x               | 1; 6; 7  |
| 547                                | 193        | 207      | YQEPVLGPVRGPFPPI   | none         | 2     | 834.961 | 55.25                | 3.8   | 83.1   | x               | x                 | x               | 7  |
| 548                                | 193        | 208      | YQEPVLGPVRGPFPPII  | none         | 2     | 891.501 | 60.09                | 4.1   | 85.1   | x               | x                 | x               | 1; 5   |
| 549                                | 193        | 209      | YQEPVLGPVRGPFPPIV  | none         | 2 (3) | 941.035 | 62.19                | 3.8   | 91.8   | x               | x                 | x               | 1; 5; 6  |
| 550                                | 194        | 202      | QEPVLGPVR          | none         | 2     | 497.787 | 26.58                | 2.0   | 41.2   | x               | x                 |                 | 1  |
| 551                                | 194        | 206      | QEPVLGPVRGPFP      | none         | 2     | 696.884 | 45.81                | 2.8   | 66.0   | x               | x                 | x               | 1; 5; 7  |
| 552                                | 194        | 208      | QEPVLGPVRGPFPPI    | none         | 2     | 809.969 | 58.45                | 2.9   | 72.1   | x               | x                 | x               | 1; 5; 7  |
| 553                                | 194        | 209      | QEPVLGPVRGPFPPIV   | none         | 2     | 859.503 | 60.57                | 3.1   | 77.1   | x               | x                 | x               | 1; 5   |
| 554                                | 195        | 206      | EPVLGPVRGPFP       | none         | 2     | 632.855 | 45.94                | 2.5   | 61.7   | x               | x                 | x               | 1; 4; 5; 6; 7  |
| 555                                | 195        | 207      | EPVLGPVRGPFPPI     | none         | 2     | 689.398 | 53.30                | 2.1   | 47.3   | x               | x                 | x               | 1; 5; 7  |
| 556                                | 195        | 208      | EPVLGPVRGPFPPII    | none         | 2     | 745.940 | 58.53                | 2.6   | 62.8   | x               | x                 | x               | 1; 5   |
| 557                                | 195        | 209      | EPVLGPVRGPFPPIV    | none         | 2     | 795.474 | 60.82                | 2.7   | 66.9   | x               | x                 | x               | 1; 2; 4; 5   |
| 558                                | 196        | 209      | PVLGPVRGPFPPIV     | none         | 2     | 730.953 | 60.32                | 3.1   | 65.3   | x               | x                 | x               | 1; 3   |
| 559                                | 197        | 209      | VLGPVRGPFPPIV      | none         | 2     | 682.427 | 58.12                | 1.9   | 46.5   |                 | x                 | x               |  |
| 560                                | 198        | 209      | LGPVRGPFPPIV       | none         | 2     | 632.892 | 56.47                | 1.8   | 46.8   | x               | x                 | x               | 5  |
| 561                                | 199        | 208      | GPVRGPFPPII        | none         | 2     | 526.815 | 48.58                | 2.1   | 46.6   | x               | x                 | x               | 1  |
| 562                                | 199        | 209      | GPVRGPFPPIIV       | none         | 2     | 576.350 | 51.83                | 1.7   | 43.6   | x               | x                 | x               | 1; 4; 5  |
| 563                                | 200        | 209      | PVRGPFPPIIV        | none         | 2     | 547.837 | 51.65                | 2.1   | 36.0   | x               | x                 | x               | 1; 2; 6  |
| <b>Beta-lactoglobulin (P02754)</b> |            |          |                    |              |       |         |                      |       |        |                 |                   |                 |  |
| 564                                | 1          | 8        | LIVTQTMK           | none         | 2     | 467.274 | 25.46                | 2.4   | 48.2   | x               | x                 | x               | 1; 2   |
| 565                                | 1          | 10       | LIVTQTMKGL         | none         | 2     | 552.328 | 40.43                | 2.7   | 55.7   |                 | x                 | x               |  |
| 566                                | 1          | 10       | LIVTQTMKGL         | M7(Ox)       | 2     | 560.326 | 30.39                | 2.3   | 56.8   |                 |                   | x               |  |
| 567                                | 1          | 11       | LIVTQTMKGLD        | none         | 2     | 609.843 | 37.95                | 3.3   | 71.7   | x               | x                 |                 |  |
| 568                                | 1          | 11       | LIVTQTMKGLD        | M7(Ox)       | 2     | 617.840 | 28.49                | 2.7   | 69.5   | x               | x                 |                 |  |
| 569                                | 1          | 13       | LIVTQTMKGLDIQ      | none         | 2     | 730.415 | 45.62                | 3.6   | 80.9   | x               | x                 |                 |  |

| Nr.  | Start pos. | End pos. | Sequence                | Modification | z       | m/z     | t <sub>r</sub> (min) | Xcorr | -10lgP | RM <sup>a</sup> | UH T <sup>a</sup> | IF <sup>a</sup> | Literature (milk <sup>1-6</sup> , colostrum <sup>7</sup> ) |
|--|------------|----------|-------------------------|--------------|---------|---------|----------------------|-------|--------|-----------------|-------------------|-----------------|--|
| 570  | 1          | 13       | LIVTQTmKGLDIQ           | M7(Ox)       | 2       | 738.412 | 37.26                | 3.3   | 72.2   |                 | x                 | x               |  |
| 571  | 1          | 17       | LIVTQTMKGLDIQKVAG       | none         | 2       | 908.025 | 44.70                | 3.4   | 51.7   | x               | x                 |                 |  |
| 572  | 2          | 13       | IVTQTMKGLDIQ            | none         | 2       | 673.872 | 36.76                | 2.6   | 51.5   |                 | x                 |                 |  |
| 573  | 9          | 16       | GLDIQKVA                | none         | 2       | 422.250 | 29.83                | 2.0   | 37.7   |                 | x                 |                 |  |
| 574  | 9          | 22       | GLDIQKVAGTWYSL          | none         | 2       | 775.914 | 58.01                | 3.2   | 68.3   |                 | x                 |                 |  |
| 575  | 11         | 22       | DIQKVAGTWYSL            | none         | 2       | 690.863 | 49.95                | 3.6   | 60.5   |                 | x                 |                 |  |
| 576  | 14         | 22       | KVAGTWYSL               | none         | 2       | 512.776 | 41.72                | 2.3   | 61.5   |                 | x                 |                 |  |
| 577  | 33         | 42       | DAQSAPLRVY              | none         | 2       | 560.292 | 30.72                | 2.6   | 76.1   |                 | x                 |                 |  |
| 578  | 127        | 136      | EVDDEALEKF              | none         | 2       | 597.779 | 37.48                | 2.0   | 36.0   | x               | x                 |                 |  |
| 579  | 153        | 162      | PTQLEEQCHI              | none         | 2       | 599.281 | 29.13                | 3.0   | 63.5   | x               | x                 |                 |  |
| <b>Butyrophilin subfamily 1 member A1 (P18892)</b> |            |          |                         |              |         |         |                      |       |        |                 |                   |                 |  |
| 580  | 50         | 66       | VSREGQEQQEGEEMAAYR      | none         | 3 (2)   | 676.297 | 24.37                | 5.4   | 103.8  | x               | x                 | x               |  |
| 581  | 50         | 66       | VSREGQEQQEGEEmAEYR      | M13(Ox)      | 3 (2)   | 681.629 | 18.02                | 5.3   | 69.8   | x               | x                 | x               |  |
| 582  | 53         | 66       | EGQEQQEGEEMAAYR         | none         | 2       | 842.840 | 26.18                | 3.7   | 70.2   | x               | x                 | x               |  |
| 583  | 53         | 66       | EGQEQQEGEEmAEYR         | M10(Ox)      | 2       | 850.838 | 18.52                | 2.7   | 48.9   | x               | x                 |                 |  |
| 584  | 67         | 84       | GRVSLVEDHIAEGSVAVR      | none         | 3 (4)   | 632.009 | 33.19                | 4.0   | 67.8   | x               | x                 | x               |  |
| 585  | 68         | 84       | RVSLVEDHIAEGSVAVR       | none         | 3       | 613.001 | 32.41                | 3.7   | 55.1   | x               | x                 | x               |  |
| 586  | 69         | 84       | VSLVEDHIAEGSVAVR        | none         | 3       | 560.969 | 35.23                | 4.0   | 65.0   | x               | x                 | x               |  |
| 587  | 70         | 84       | SLVEDHIAEGSVAVR         | none         | 3 (2)   | 527.945 | 32.36                | 3.9   | 77.3   | x               | x                 |                 |  |
| 588  | 72         | 82       | VEDHIAEGSVA             | none         | 2       | 563.770 | 22.24                | 2.1   | 47.6   | x               | x                 | x               |  |
| 589  | 72         | 84       | VEDHIAEGSVAVR           | none         | 3 (2)   | 461.240 | 23.63                | 4.3   | 66.3   | x               | x                 | x               |  |
| 590  | 85         | 97       | IQEVKASDDGEYR           | none         | 2       | 755.361 | 19.00                | 3.6   | 63.5   | x               | x                 |                 |  |
| 591  | 102        | 114      | QDENYEEAIVHLK           | none         | 3       | 529.924 | 37.79                | 3.3   | 35.8   | x               | x                 |                 |  |
| 592  | 153        | 177      | THRGEFPMSESRNPDEEGLFTVR | none         | 4 (3,5) | 727.589 | 39.91                | 5.9   | 89.2   | x               | x                 | x               | 3; 5   |
| 593  | 153        | 177      | THRGEFPMSesRNPDEEGLFTVR | M10(Ox)      | 4 (3,5) | 731.586 | 34.95                | 5.4   | 54.7   | x               | x                 | x               | 3  |
| 594  | 156        | 177      | GEEFPMSesRNPDEEGLFTVR   | none         | 3       | 838.380 | 45.95                | 4.8   | 65.2   | x               | x                 | x               |  |
| 595  | 169        | 177      | DEEGLFTVR               | none         | 2       | 533.263 | 38.33                | 2.6   | 54.1   |                 | x                 |                 |  |
| 596  | 196        | 203      | NLLLGQEK                | none         | 2       | 457.767 | 27.71                | 2.2   | 31.5   | x               | x                 |                 |  |
| 597  | 287        | 297      | PHHLFLYEDSK             | none         | 3       | 462.564 | 31.26                | 3.4   | 60.7   | x               | x                 |                 |  |

| Nr.  | Start pos. | End pos. | Sequence                          | Modification | z         | m/z      | t <sub>r</sub> (min) | Xcorr | -10lgP | RM <sup>a</sup> | UH T <sup>a</sup> | IF <sup>a</sup> | Literature (milk <sup>1-6</sup> , colostrum <sup>7</sup> ) |
|--|------------|----------|-----------------------------------|--------------|-----------|----------|----------------------|-------|--------|-----------------|-------------------|-----------------|--|
| 598  | 467        | 500      | KEIPLSPMGEDSASGDIETLHSKLIPLQPSQGV | none         | 3         | 1190.953 | 53.65                | 4.3   | 48.0   | x               | x                 |                 |  |
| 599  | 469        | 487      | IPLSPMGEDSASGDIETLH               | none         | 2         | 984.967  | 43.78                | 5.5   | 123.4  | x               | x                 | x               | 5  |
| 600  | 469        | 487      | IPLSPmGEDSASGDIETLH               | M6(Ox)       | 2         | 992.963  | 38.58                | 5.0   | 99.5   | x               | x                 | x               |  |
| 601  | 472        | 487      | SPmGEDSASGDIETLH                  | M3(Ox)       | 2         | 831.350  | 27.44                | 3.3   | 68.5   | x               | x                 | x               |  |
| 602  | 475        | 487      | GEDSASGDIETLH                     | none         | 2         | 665.789  | 25.58                | 3.7   | 84.0   | x               | x                 | x               |  |
| <b>CCAAT/enhancer-binding protein beta (O02755)</b>                        |            |          |                                   |              |           |          |                      |       |        |                 |                   |                 |  |
| 603  | 161        | 169      | HPPPPPPP                          | none         | 2         | 466.751  | 18.19                | 2.2   | 48.0   | x               | x                 |                 |  |
| <b>DNA-directed RNA polymerases I, II, and III subunit RPABC1 (Q2T9T3)</b> |            |          |                                   |              |           |          |                      |       |        |                 |                   |                 |  |
| 604  | 77         | 87       | PEEPKVGIKTI                       | none         | 3 (2)     | 404.239  | 29.20                | 3.2   | 53.8   | x               | x                 |                 |  |
| <b>DnaJ homolog subfamily C member 12 (Q9N287)</b>                         |            |          |                                   |              |           |          |                      |       |        |                 |                   |                 |  |
| 605  | 185        | 193      | APSELLRKF                         | none         | 2         | 530.811  | 34.61                | 2.8   | 45.6   | x               | x                 |                 |  |
| <b>Fatty acid synthase (Q71SP7)</b>  |            |          |                                   |              |           |          |                      |       |        |                 |                   |                 |  |
| 606  | 379        | 389      | RPLPVLGNNVG                       | none         | 2         | 539.821  | 36.20                | 2.6   | 53.8   | x               | x                 |                 |  |
| 607  | 379        | 393      | RPLPVLGNNVGINSF                   | none         | 2         | 770.435  | 51.61                | 3.1   | 58.6   | x               | x                 |                 |  |
| 608  | 1483       | 1493     | SPIPETDPKSL                       | none         | 2         | 592.313  | 31.30                | 2.4   | 61.1   | x               | x                 | x               |  |
| 609  | 20         | 38       | EDGSDPPSGDFLTEGGGVR               | none         | 2         | 946.420  | 37.27                | 3.3   | 87.9   | x               | x                 | x               |  |
| <b>Fibroblast growth factor-binding protein 1 (Q9MZ06)</b>                 |            |          |                                   |              |           |          |                      |       |        |                 |                   |                 |  |
| 610  | 8          | 27       | RGSKASADESALGKPGKEP               | none         | 4         | 500.269  | 22.06                | 2.7   | 32.2   | x               | x                 | x               |  |
| 611  | 8          | 28       | RGSKASADESALGKPGKEPR              | none         | 4 (5)     | 539.295  | 19.29                | 5.0   | 70.4   | x               | x                 | x               | 2; 5   |
| 612  | 9          | 27       | GSKASADESALGKPGKEP                | none         | 3         | 614.655  | 24.30                | 4.5   | 59.0   | x               | x                 | x               |  |
| 613  | 9          | 28       | GSKASADESALGKPGKEPR               | none         | 3 (2,4,5) | 666.691  | 20.88                | 3.8   | 55.0   | x               | x                 | x               | 2; 3; 5  |
| 614  | 9          | 28       | GSKAsADESALGKPGKEPR               | S5(Phospho)  | 4         | 520.261  | 22.73                | 4.1   | 31.4   | x               | x                 |                 | 3  |
| 615  | 12         | 28       | ASADESALGKPGKEPR                  | none         | 3 (4)     | 575.976  | 22.88                | 3.7   | 55.9   | x               | x                 | x               | 5  |
| 616  | 13         | 28       | SADESALGKPGKEPR                   | none         | 3         | 552.295  | 22.11                | 3.6   | 36.6   | x               | x                 |                 |  |
| 617  | 14         | 28       | ADESLALGKPGKEPR                   | none         | 3         | 523.285  | 21.58                | 3.1   | 29.9   | x               | x                 |                 |  |
| <b>FXYD domain-containing ion transport regulator 6 (Q3MHZ5)</b>           |            |          |                                   |              |           |          |                      |       |        |                 |                   |                 |  |
| 618  | 1          | 20       | SATEQEKEKDPFHODYQTTLR             | none         | 4 (3)     | 622.046  | 32.90                | 3.4   | 42.2   | x               | x                 | x               |  |
| 619  | 1          | 25       | SATEQEKEKDPFHODYQTLRIGGLV         | none         | 3 (4)     | 975.486  | 49.06                | 4.6   | 76.6   | x               | x                 | x               |  |
| <b>Glycosylation-dependent cell adhesion molecule 1 (P80195)</b>           |            |          |                                   |              |           |          |                      |       |        |                 |                   |                 |  |

| Nr. | Start pos. | End pos. | Sequence  | Modification | z       | m/z      | t <sub>r</sub> (min) | Xcorr | -10lgP | RM <sup>a</sup> | UH T <sup>a</sup> | IF <sup>a</sup> | Literature (milk <sup>1-6</sup> , colostrum <sup>7</sup> ) |
|-----|------------|----------|---|--------------|---------|----------|----------------------|-------|--------|-----------------|-------------------|-----------------|--|
| 620 | 1          | 11       | ILNKPEDETHL   | none         | 2 (3)   | 654.843  | 25.37                | 3.4   | 73.6   |                 | x                 | x               |  |
| 621 | 1          | 12       | ILNKPEDETHLE  | none         | 2 (3)   | 719.364  | 24.28                | 3.7   | 71.4   | x               | x                 | x               |  |
| 622 | 1          | 16       | ILNKPEDETHLEAQPT  | none         | 2       | 917.964  | 26.34                | 3.3   | 71.8   | x               | x                 | x               |  |
| 623 | 1          | 17       | ILNKPEDETHLEAQPTD   | none         | 2       | 975.475  | 26.66                | 4.4   | 73.7   | x               | x                 | x               |  |
| 624 | 1          | 18       | ILNKPEDETHLEAQPTDA  | none         | 3 (2)   | 674.332  | 27.78                | 2.3   | 47.4   | x               | x                 | x               |  |
| 625 | 1          | 20       | ILNKPEDETHLEAQPTDASA                                      | none         | 2       | 1090.030 | 28.01                | 3.7   | 58.1   | x               | x                 | x               | 3  |
| 626 | 1          | 21       | ILNKPEDETHLEAQPTDASAQ                                     | none         | 2 (3)   | 1154.065 | 27.25                | 3.3   | 71.3   | x               | x                 | x               | 7  |
| 627 | 1          | 22       | ILNKPEDETHLEAQPTDASAQF                                    | none         | 2 (3)   | 1227.595 | 35.72                | 4.8   | 105.5  | x               | x                 | x               | 3; 5; 7  |
| 628 | 1          | 23       | ILNKPEDETHLEAQPTDASAQFI                                   | none         | 2 (3)   | 1284.141 | 41.00                | 3.6   | 60.9   | x               | x                 | x               | 5  |
| 629 | 1          | 24       | ILNKPEDETHLEAQPTDASAQFIR                                  | none         | 3 (2,4) | 908.460  | 36.52                | 6.1   | 99.0   | x               | x                 | x               | 3; 5   |
| 630 | 1          | 24       | ILNKPEDETHLEAQPTDAsAQFIR                                  | S19(Phospho) | 3       | 935.114  | 36.44                | 4.9   | 51.7   | x               | x                 | x               |  |
| 631 | 1          | 25       | ILNKPEDETHLEAQPTDASAQFIRN                                 | none         | 3       | 946.474  | 35.84                | 6.2   | 73.4   | x               | x                 | x               | 3; 4; 5  |
| 632 | 1          | 26       | ILNKPEDETHLEAQPTDASAQFIRNL                                | none         | 3 (4)   | 984.169  | 47.12                | 7.4   | 94.4   | x               | x                 | x               |  |
| 633 | 1          | 27       | ILNKPEDETHLEAQPTDASAQFIRNLQ                               | none         | 3 (4)   | 1026.855 | 44.88                | 6.2   | 86.5   | x               | x                 | x               | 5  |
| 634 | 1          | 53       | ILNKPEDETHLEAQPTDASAQFIRNLQISNEDLSKEPSISREDLI<br>SKEQIVIR | none         | 6 (5)   | 1010.530 | 54.54                | 5.3   | 30.0   | x               | x                 | x               |  |
| 635 | 2          | 12       | LNKPEDETHLE   | none         | 3 (2)   | 442.217  | 20.37                | 3.2   | 65.4   | x               | x                 | x               |  |
| 636 | 2          | 22       | LNKPEDETHLEAQPTDASAQF                                     | none         | 3 (2)   | 781.038  | 33.47                | 4.4   | 71.4   | x               | x                 | x               | 7  |
| 637 | 2          | 24       | LNKPEDETHLEAQPTDASAQFIR                                   | none         | 4       | 653.324  | 34.72                | 3.8   | 44.2   | x               | x                 | x               | 5  |
| 638 | 12         | 22       | EAQPTDASAQF   | none         | 2       | 582.761  | 27.79                | 2.8   | 73.9   |                 |                   | x               |  |
| 639 | 13         | 22       | AQPTDASAQF  | none         | 2       | 518.240  | 26.40                | 2.6   | 52.4   |                 |                   | x               |  |
| 640 | 13         | 26       | AQPTDASAQFIRNL  | none         | 2       | 766.397  | 46.18                | 3.1   | 75.8   |                 |                   | x               |  |
| 641 | 44         | 53       | LlsKEQIVIR  | S3(Phospho)  | 2       | 639.862  | 35.70                | 3.2   | 44.0   | x               | x                 | x               |  |
| 642 | 54         | 66       | SSRQPQSQNPKLP   | none         | 3       | 489.594  | 19.71                | 2.9   | 45.8   | x               | x                 | x               |  |
| 643 | 54         | 67       | SSRQPQSQNPKLPL  | none         | 3 (2)   | 527.289  | 27.77                | 3.5   | 60.7   | x               | x                 | x               |  |
| 644 | 54         | 68       | SSRQPQSQNPKLPLS   | none         | 3 (2)   | 556.300  | 25.69                | 2.7   | 49.7   | x               | x                 | x               | 3; 5; 7  |
| 645 | 54         | 70       | SSRQPQSQNPKLPLSIL   | none         | 2 (3)   | 947.033  | 45.70                | 3.2   | 77.8   | x               | x                 | x               | 5; 7   |
| 646 | 54         | 71       | SSRQPQSQNPKLPLSILK  | none         | 3 (2,4) | 674.387  | 37.70                | 5.4   | 71.1   | x               | x                 | x               | 5  |
| 647 | 54         | 72       | SSRQPQSQNPKLPLSILKE                                       | none         | 4 (3)   | 538.303  | 39.06                | 4.8   | 61.0   | x               | x                 | x               | 3; 5   |

| Nr. | Start pos. | End pos. | Sequence               | Modification | z       | m/z     | t <sub>r</sub> (min) | Xcorr | -10lgP | RM <sup>a</sup> | UH T <sup>a</sup> | IF <sup>a</sup> | Literature (milk <sup>1-6</sup> , colostrum <sup>7</sup> ) |
|-----|------------|----------|------------------------|--------------|---------|---------|----------------------|-------|--------|-----------------|-------------------|-----------------|--|
| 648 | 54         | 73       | SSRQPQSQNPKLPLSILKEK   | none         | 4 (3,5) | 570.327 | 34.40                | 5.8   | 59.2   | x               | x                 | x               | 2; 3; 5  |
| 649 | 54         | 75       | SSRQPQSQNPKLPLSILKEKHL | none         | 4 (3,5) | 632.862 | 36.82                | 5.2   | 55.9   | x               | x                 | x               | 2; 3; 5  |
| 650 | 55         | 68       | SRQPQSQNPKLPLS         | none         | 3 (2)   | 527.289 | 25.48                | 2.8   | 38.5   | x               | x                 | x               | 3; 5   |
| 651 | 55         | 70       | SRQPQSQNPKLPLSIL       | none         | 3       | 602.680 | 45.70                | 3.0   | 24.8   | x               | x                 | x               |  |
| 652 | 55         | 71       | SRQPQSQNPKLPLSILK      | none         | 4 (3)   | 484.284 | 37.75                | 4.1   | 60.2   | x               | x                 | x               |  |
| 653 | 57         | 68       | QPQSQNPKLPLS           | none         | 2       | 668.864 | 28.63                | 2.1   | 55.3   | x               | x                 | x               | 5  |
| 654 | 57         | 70       | QPQSQNPKLPLSIL         | none         | 2       | 781.948 | 50.34                | 1.9   | 52.9   | x               | x                 | x               | 5  |
| 655 | 57         | 71       | QPQSQNPKLPLSILK        | none         | 3       | 564.333 | 41.21                | 1.8   | 30.6   | x               | x                 |                 |  |
| 656 | 57         | 73       | QPQSQNPKLPLSILKEK      | none         | 3 (4)   | 650.046 | 37.29                | 3.1   | 26.5   | x               | x                 | x               | 5  |
| 657 | 57         | 75       | QPQSQNPKLPLSILKEKHL    | none         | 3 (5)   | 733.426 | 39.24                | 2.3   | 37.1   | x               | x                 |                 | 5  |
| 658 | 60         | 67       | SQNPKLPL               | none         | 2       | 448.763 | 30.54                | 2.1   | 42.0   |                 |                   | x               |  |
| 659 | 60         | 68       | SQNPKLPLS              | none         | 2       | 492.279 | 27.81                | 2.0   | 45.6   |                 |                   | x               |  |
| 660 | 60         | 70       | SQNPKLPLSIL            | none         | 2       | 605.364 | 50.30                | 2.4   | 51.9   |                 |                   | x               | 7  |
| 661 | 62         | 70       | NPKLPLSIL              | none         | 2       | 497.818 | 51.03                | 2.2   | 35.4   |                 |                   | x               |  |
| 662 | 63         | 70       | PKLPLSIL               | none         | 2       | 440.797 | 50.94                | 1.9   | 25.4   |                 |                   | x               |  |
| 663 | 65         | 73       | LPLSILKEK              | none         | 2       | 520.839 | 35.61                | 1.8   | 43.7   | x               | x                 |                 | 3  |
| 664 | 65         | 74       | LPLSILKEKH             | none         | 2       | 589.368 | 31.08                | 2.2   | 47.5   | x               | x                 |                 |  |
| 665 | 65         | 75       | LPLSILKEKHL            | none         | 2 (3)   | 645.910 | 37.83                | 3.5   | 55.1   | x               | x                 | x               |  |
| 666 | 109        | 121      | RNLENTVKETIKY          | none         | 3 (2)   | 536.629 | 32.85                | 4.0   | 61.3   | x               | x                 |                 |  |
| 667 | 111        | 121      | LENTVKETIKY            | none         | 2 (3)   | 669.369 | 27.69                | 3.2   | 66.8   |                 |                   | x               |  |
| 668 | 112        | 121      | ENTVKETIKY             | none         | 2 (3)   | 612.827 | 23.24                | 2.9   | 47.2   |                 |                   | x               |  |
| 669 | 113        | 121      | NTVKETIKY              | none         | 2       | 548.305 | 21.05                | 2.3   | 46.5   |                 |                   | x               |  |
| 670 | 122        | 135      | LKSLFSHAFEVVKT         | none         | 3 (4)   | 535.972 | 43.57                | 3.2   | 70.5   |                 |                   | x               |  |
| 671 | 123        | 135      | KSLFSHAFEVVKT          | none         | 3       | 498.276 | 39.18                | 3.5   | 50.7   |                 |                   | x               |  |
| 672 | 124        | 135      | SLFSHAFEVVKT           | none         | 2       | 682.864 | 46.16                | 3.2   | 79.8   | x               | x                 |                 |  |
| 673 | 126        | 135      | FSHAFEVVKT             | none         | 2       | 582.805 | 30.31                | 2.6   | 73.2   |                 |                   | x               |  |
| 674 | 127        | 135      | SHAFEVVKT              | none         | 2       | 509.270 | 22.60                | 2.9   | 73.2   | x               | x                 | x               | 3; 5   |
| 675 | 128        | 135      | HAFEVVKT               | none         | 2       | 465.755 | 21.45                | 2.2   | 55.9   | x               | x                 | x               |  |

Kappa-casein (P02668)

| Nr. | Start pos. | End pos. | Sequence   | Modification | z | m/z      | t <sub>r</sub> (min) | Xcorr | -10lgP | RM <sup>a</sup> | UH T <sup>a</sup> | IF <sup>a</sup> | Literature (milk <sup>1-6</sup> , colostrum <sup>7</sup> ) |
|-----|------------|----------|--|--------------|---|----------|----------------------|-------|--------|-----------------|-------------------|-----------------|--|
| 676 | 14         | 24       | DERFFSDKIAK  | none         | 3 | 452.569  | 29.31                | 3.4   | 41.0   | x               | x                 | x               |  |
| 677 | 31         | 38       | VLSRYPSY   | none         | 2 | 492.761  | 26.80                | 2.4   | 58.3   |                 |                   | x               |  |
| 678 | 31         | 40       | VLSRYPSYGL   | none         | 2 | 577.813  | 36.76                | 2.7   | 65.7   |                 |                   | x               |  |
| 679 | 31         | 41       | VLSRYPSYGLN  | none         | 2 | 634.836  | 32.74                | 3.1   | 73.5   |                 |                   | x               |  |
| 680 | 31         | 43       | VLSRYPSYGLNYY  | none         | 2 | 797.901  | 42.57                | 2.8   | 65.6   |                 |                   | x               |  |
| 681 | 33         | 40       | SRYPSYGL   | none         | 2 | 471.736  | 30.91                | 2.2   | 47.8   |                 |                   | x               |  |
| 682 | 33         | 41       | SRYPSYGLN  | none         | 2 | 528.759  | 26.99                | 2.5   | 62.1   |                 |                   | x               |  |
| 683 | 33         | 43       | SRYPSYGLNYY  | none         | 2 | 691.824  | 38.76                | 3.4   | 63.3   |                 |                   | x               |  |
| 684 | 41         | 50       | NYQQQKPVAL   | none         | 2 | 612.325  | 31.29                | 2.8   | 67.2   |                 |                   | x               |  |
| 685 | 42         | 50       | YYQQQKPVAL   | none         | 2 | 555.303  | 28.59                | 2.7   | 58.1   |                 |                   | x               | 7  |
| 686 | 42         | 53       | YYQQQKPVALINN  | none         | 2 | 725.889  | 31.23                | 3.4   | 50.9   |                 |                   | x               |  |
| 687 | 43         | 50       | YQQQKPVAL  | none         | 2 | 473.770  | 24.17                | 2.4   | 47.3   |                 |                   | x               |  |
| 688 | 43         | 53       | YQQQKPVALINN   | none         | 2 | 644.356  | 27.79                | 3.2   | 45.1   |                 |                   | x               |  |
| 689 | 49         | 65       | ALINNQFLPYPPYYAKPA   | none         | 2 | 992.023  | 53.06                | 3.4   | 55.7   | x               | x                 |                 | 5  |
| 690 | 51         | 65       | INNQFLPYPPYYAKPA   | none         | 2 | 899.963  | 46.66                | 4.2   | 65.6   |                 |                   | x               |  |
| 691 | 52         | 65       | NNQFLPYPPYYAKPA  | none         | 2 | 843.421  | 44.60                | 2.9   | 59.9   |                 |                   | x               |  |
| 692 | 66         | 74       | AVRSPAQIL  | none         | 2 | 477.790  | 33.35                | 2.2   | 36.9   |                 |                   | x               |  |
| 693 | 66         | 76       | AVRSPAQILQW  | none         | 2 | 634.860  | 49.07                | 2.1   | 49.7   |                 |                   | x               |  |
| 694 | 69         | 79       | SPAQILQWQVL  | none         | 2 | 641.862  | 61.49                | 1.6   | 54.8   | x               |                   |                 | 5  |
| 695 | 106        | 137      | MAIPPKKNQDKTEIPTINTIASGEPTSTPTTE                                     | none         | 4 | 853.441  | 38.57                | 2.9   | 31.8   |                 |                   | x               |  |
| 696 | 106        | 137      | mAIPPKKNQDKTEIPTINTIASGEPTSTPTTE                                     | M1(Ox)       | 4 | 857.439  | 37.24                | 4.1   | 25.9   |                 |                   | x               |  |
| 697 | 106        | 169      | MAIPPKKNQDKTEIPTINTIASGEPTSTPTTEAVESTVATLEDsP<br>EVIESPPEINTVQVTSTAV | S44(Phospho) | 4 | 1696.848 | 62.56                | 3.8   | 26.3   |                 |                   | x               |  |
| 698 | 114        | 123      | QDKTEIPTIN   | none         | 2 | 579.803  | 29.01                | 2.1   | 41.2   |                 |                   | x               |  |
| 699 | 148        | 169      | DsPEVIESPPEINTVQVTSTAV   | S2(Phospho)  | 2 | 1196.565 | 53.71                | 3.8   | 59.2   |                 | x                 | x               |  |
| 700 | 149        | 169      | SPEVIESPPEINTVQVTSTAV  | none         | 2 | 1099.067 | 48.66                | 4.2   | 98.1   | x               | x                 | x               |  |
| 701 | 149        | 169      | sPEVIESPPEINTVQVTSTAV  | S1(Phospho)  | 2 | 1139.050 | 52.01                | 4.3   | 82.7   | x               | x                 | x               |  |
| 702 | 150        | 169      | PEVIESPPEINTVQVTSTAV   | none         | 2 | 1055.551 | 48.60                | 4.1   | 90.8   | x               | x                 | x               |  |
| 703 | 151        | 169      | EVIESPPEINTVQVTSTAV  | none         | 2 | 1007.024 | 47.36                | 3.1   | 68.6   |                 | x                 | x               |  |

| Nr.  | Start pos. | End pos. | Sequence             | Modification | z     | m/z      | t <sub>r</sub> (min) | Xcorr | -10lgP | RM <sup>a</sup> | UH T <sup>a</sup> | IF <sup>a</sup> | Literature (milk <sup>1-6</sup> , colostrum <sup>7</sup> ) |
|--|------------|----------|----------------------|--------------|-------|----------|----------------------|-------|--------|-----------------|-------------------|-----------------|--|
| 704  | 152        | 160      | VIESPPEIN            | none         | 2     | 499.263  | 30.82                | 2.5   | 62.2   |                 | x                 | x               |  |
| 705  | 152        | 161      | VIESPPEINT           | none         | 2     | 549.787  | 33.18                | 2.4   | 56.9   | x               | x                 | x               | 7  |
| 706  | 152        | 169      | VIESPPEINTVQVTSTAV   | none         | 2     | 942.502  | 45.84                | 2.9   | 64.9   |                 | x                 | x               |  |
| 707  | 155        | 169      | SPPEINTVQVTSTAV      | none         | 2     | 771.905  | 40.01                | 2.3   | 65.2   |                 | x                 | x               |  |
| 708  | 159        | 169      | INTVQVTSTAV          | none         | 2     | 566.813  | 33.08                | 2.4   | 57.2   |                 | x                 | x               | 1; 7   |
| 709  | 161        | 169      | TVQVTSTAV            | none         | 2     | 453.249  | 25.67                | 2.6   | 51.5   |                 | x                 | x               | 3  |
| <b>Lactoperoxidase (P80025)</b>                                  |            |          |                      |              |       |          |                      |       |        |                 |                   |                 |  |
| 710  | 1          | 20       | DTIAQAASTTIISDAVSKVK | none         | 2 (3) | 1004.034 | 42.63                | 4.3   | 73.2   | x               | x                 | x               |  |
| 711  | 35         | 46       | KTTLSEAPTTQ          | none         | 2     | 632.325  | 17.99                | 2.4   | 63.4   |                 |                   | x               |  |
| 712  | 37         | 53       | TLSSEAPTTQQLSEYFK    | none         | 2     | 965.476  | 47.25                | 5.0   | 93.2   | x               | x                 |                 |  |
| 713  | 39         | 51       | SSEAPTTQQLSEY        | none         | 2     | 720.829  | 32.42                | 2.6   | 75.0   |                 |                   | x               |  |
| 714  | 40         | 51       | SEAPTTQQLSEY         | none         | 2     | 677.312  | 32.40                | 2.1   | 47.2   |                 |                   | x               |  |
| 715  | 61         | 74       | TAIRNGQVWEESLK       | none         | 3     | 544.289  | 32.63                | 3.4   | 55.2   | x               | x                 | x               | 5  |
| 716  | 61         | 76       | TAIRNGQVWEESLKRL     | none         | 4 (3) | 475.765  | 41.47                | 5.2   | 61.8   | x               | x                 | x               |  |
| 717  | 62         | 74       | AIRNGQVWEESLK        | none         | 3     | 510.606  | 31.57                | 3.9   | 40.9   | x               | x                 | x               | 3  |
| 718  | 62         | 76       | AIRNGQVWEESLKRL      | none         | 4     | 450.502  | 40.52                | 3.3   | 24.9   | x               | x                 | x               |  |
| 719  | 65         | 74       | NGQVWEESLK           | none         | 2     | 595.296  | 32.68                | 2.1   | 53.4   | x               | x                 | x               | 3  |
| 720  | 66         | 74       | GQVWEESLK            | none         | 2     | 538.274  | 32.27                | 2.8   | 53.1   | x               | x                 | x               | 5  |
| 721  | 66         | 76       | GQVWEESLKRL          | none         | 2 (3) | 672.866  | 41.64                | 3.2   | 57.6   | x               | x                 | x               |  |
| 722  | 67         | 74       | QVWEESLK             | none         | 2     | 509.763  | 30.34                | 1.6   | 38.3   | x               | x                 | x               |  |
| 723  | 67         | 76       | QVWEESLKRL           | none         | 2 (3) | 429.906  | 39.35                | 1.8   | 54.1   | x               | x                 | x               | 2  |
| 724  | 68         | 76       | VWEESLKRL            | none         | 2     | 580.327  | 35.46                | 2.4   | 53.4   | x               | x                 | x               |  |
| <b>Wiskott-Aldrich syndrome protein family member 2 (A2VDK6)</b> |            |          |                      |              |       |          |                      |       |        |                 |                   |                 |  |
| 725  | 384        | 393      | APP PPPPPP           | none         | 2     | 482.267  | 24.04                | 2.8   | 45.9   | x               | x                 |                 |  |
| 726  | 385        | 393      | PPP PPPPPP           | none         | 2     | 446.748  | 23.87                | 2.1   | 41.1   | x               | x                 | x               |  |
| 727  | 385        | 393      | PPPPP PPPPP          | none         | 2     | 495.274  | 25.65                | 2.4   | 41.2   | x               | x                 | x               |  |
| <b>Mucin-1 (Q8WML4)</b>  |            |          |                      |              |       |          |                      |       |        |                 |                   |                 |  |
| 728  | 532        | 545      | SPYEEVSAGNGGSN       | none         | 2     | 684.288  | 22.52                | 2.5   | 41.8   | x               | x                 |                 |  |
| <b>Mucin-15 (Q8MI01)</b>   |            |          |                      |              |       |          |                      |       |        |                 |                   |                 |  |

| Nr.   | Start pos. | End pos. | Sequence                   | Modification | z     | m/z     | t <sub>r</sub> (min) | Xcorr | -10lgP | RM <sup>a</sup> | UH T <sup>a</sup> | IF <sup>a</sup> | Literature (milk <sup>1-6</sup> , colostrum <sup>7</sup> ) |
|---|------------|----------|----------------------------|--------------|-------|---------|----------------------|-------|--------|-----------------|-------------------|-----------------|--|
| 729   | 246        | 257      | RLYDDRNEPVLR               | none         | 3     | 515.942 | 25.09                | 2.6   | 36.3   | x               | x                 |                 |  |
| 730   | 247        | 257      | LYDDRNEPVLR                | none         | 2 (3) | 695.359 | 26.02                | 2.3   | 47.0   | x               | x                 |                 |  |
| 731   | 248        | 257      | YDDRNEPVLR                 | none         | 3     | 426.213 | 21.04                | 2.7   | 36.8   | x               | x                 | x               |  |
| <b>Myosin regulatory light polypeptide 9 (Q5E9E2)</b> |            |          |                            |              |       |         |                      |       |        |                 |                   |                 |  |
| 732   | 97         | 105      | TDPEDVIRN                  | none         | 2     | 529.758 | 24.72                | 1.8   | 45.4   | x               | x                 |                 |  |
| 733   | 98         | 105      | DPEDVIRN                   | none         | 2     | 479.234 | 22.25                | 2.5   | 47.1   | x               | x                 |                 |  |
| <b>Osteopontin (P31096)</b>                           |            |          |                            |              |       |         |                      |       |        |                 |                   |                 |  |
| 734   | 20         | 34       | YPDAVATWLKPDPSQ            | none         | 2     | 844.419 | 47.19                | 3.6   | 69.4   | x               |                   |                 |  |
| 735   | 249        | 262      | RISHELDSSASSEVN            | none         | 2     | 772.372 | 21.43                | 2.7   | 77.0   | x               | x                 | x               | 3; 5   |
| 736   | 249        | 262      | RISHELDSSAsSEVN            | S10(Phospho) | 2     | 812.352 | 21.84                | 2.8   | 45.4   | x               | x                 | x               |  |
| 737   | 249        | 262      | RISHELDsASSEVN             | S8(Phospho)  | 2     | 812.354 | 23.41                | 3.3   | 50.7   | x               | x                 | x               |  |
| 738   | 250        | 262      | ISHELDSSASSEVN             | none         | 2     | 694.319 | 22.59                | 3.2   | 64.1   | x               | x                 | x               | 3  |
| 739   | 250        | 262      | ISHELDsASSEVN              | S7(Phospho)  | 2     | 734.304 | 25.27                | 3.3   | 54.3   | x               | x                 | x               |  |
| 740   | 250        | 262      | IRILsHELDSSASSEVN          | S4(Phospho)  | 2     | 868.896 | 34.04                | 3.8   | 57.5   | x               | x                 | x               |  |
| 741   | 250        | 262      | IRISHELDsASSEVN            | S9(Phospho)  | 2     | 868.896 | 30.96                | 3.7   | 54.7   | x               | x                 | x               |  |
| 742   | 248        | 262      | IRISHELDSSAsSEVN           | S11(Phospho) | 2     | 868.896 | 29.61                | 3.2   | 52.5   | x               | x                 | x               |  |
| 743   | 251        | 262      | SHELDSSASSEVN              | none         | 2     | 637.777 | 18.34                | 2.9   | 56.8   | x               | x                 |                 |  |
| 744   | 252        | 262      | HELDSSASSEVN               | none         | 2     | 594.261 | 16.57                | 2.0   | 45.0   | x               | x                 | x               |  |
| <b>Parathyroid hormone-related protein (P58073)</b>   |            |          |                            |              |       |         |                      |       |        |                 |                   |                 |  |
| 745   | 128        | 153      | VAGTGLEEDYLSDISATsLELNSRRH | S18(Phospho) | 3 (4) | 971.795 | 49.90                | 5.1   | 30.3   |                 |                   | x               |  |
| <b>Perilipin-2 (Q9TUM6)</b>                           |            |          |                            |              |       |         |                      |       |        |                 |                   |                 |  |
| 746   | 7          | 15       | EPQLSVVTR                  | none         | 2     | 514.789 | 27.53                | 1.7   | 35.8   | x               | x                 |                 | 5  |
| 747   | 66         | 76       | LPIIQKLEPQIA               | none         | 2     | 681.920 | 47.82                | 3.4   | 61.0   | x               | x                 | x               | 5  |
| 748   | 191        | 200      | LPLTKDELEK                 | none         | 2     | 593.338 | 26.60                | 2.5   | 56.2   | x               |                   |                 |  |
| 749   | 431        | 459      | HPKPVPVSNAEGSQPDSSS        | none         | 3 (2) | 678.982 | 17.44                | 3.8   | 49.3   | x               | x                 | x               |  |
| <b>Poly(rC)-binding protein 1 (Q5E9A3)</b>            |            |          |                            |              |       |         |                      |       |        |                 |                   |                 |  |
| 750   | 317        | 327      | NPVEGSSGRQV                | none         | 2     | 565.281 | 15.67                | 2.5   | 34.4   | x               | x                 |                 |  |
| <b>Polymeric immunoglobulin receptor (P81265)</b>     |            |          |                            |              |       |         |                      |       |        |                 |                   |                 |  |
| 751   | 555        | 567      | QVKAAPAGAAIQS              | none         | 2     | 606.339 | 19.41                | 2.3   | 53.7   | x               | x                 | x               |  |

| Nr. | Start pos. | End pos. | Sequence  | Modification | z       | m/z      | t <sub>r</sub> (min) | Xcorr | -10lgP | RM <sup>a</sup> | UH T <sup>a</sup> | IF <sup>a</sup> | Literature (milk <sup>1-6</sup> , colostrum <sup>7</sup> ) |
|-----|------------|----------|---|--------------|---------|----------|----------------------|-------|--------|-----------------|-------------------|-----------------|--|
| 752 | 556        | 567      | VKAAPAGAAIQS  | none         | 2       | 542.310  | 18.18                | 2.1   | 45.5   | x               |                   |                 |  |
| 753 | 558        | 568      | AAPAGAAIQSR   | none         | 2       | 506.778  | 15.50                | 3.0   | 53.9   | x               | x                 |                 |  |
| 754 | 558        | 574      | AAPAGAAIQSRAGEIQN                                     | none         | 3 (2)   | 542.283  | 25.58                | 3.5   | 84.6   | x               | x                 | x               | 7  |
| 755 | 558        | 575      | AAPAGAAIQSRAGEIQNK                                    | none         | 2 (3)   | 876.970  | 23.89                | 4.5   | 90.0   | x               | x                 | x               | 5  |
| 756 | 559        | 573      | APAGAAIQSRAGEIQ                                       | none         | 2       | 720.382  | 25.55                | 4.5   | 78.3   | x               | x                 | x               |  |
| 757 | 559        | 574      | APAGAAIQSRAGEIQN                                      | none         | 2       | 777.405  | 24.43                | 4.4   | 82.8   | x               | x                 | x               |  |
| 758 | 559        | 575      | APAGAAIQSRAGEIQNK                                     | none         | 3       | 561.303  | 22.72                | 2.8   | 45.7   | x               | x                 |                 |  |
| 759 | 569        | 579      | AGEIQNKALLD   | none         | 2       | 586.319  | 27.50                | 2.7   | 58.2   | x               | x                 | x               |  |
| 760 | 569        | 583      | AGEIQNKALLDPSFF                                       | none         | 2       | 825.432  | 53.46                | 2.5   | 49.1   |                 |                   | x               |  |
| 761 | 569        | 613      | AGEIQNKALLDPSFFAKESVKDAAGGPGAPADPGRPTGYSGS<br>SKA     | none         | 4 (5,6) | 1105.058 | 44.24                | 4.2   | 38.5   | x               | x                 | x               |  |
| 762 | 569        | 617      | AGEIQNKALLDPSFFAKESVKDAAGGPGAPADPGRPTGYSGS<br>SKALVST | none         | 5       | 964.290  | 46.64                | 3.6   | 47.3   | x               | x                 | x               |  |
| 763 | 576        | 600      | ALLDPSFFAKESVKDAAGGPGAPAD                             | none         | 3       | 811.077  | 50.07                | 3.3   | 58.5   | x               | x                 | x               |  |
| 764 | 576        | 605      | ALLDPSFFAKESVKDAAGGPGAPADPGRPT                        | none         | 4       | 735.630  | 47.84                | 4.7   | 64.3   |                 |                   | x               |  |
| 765 | 576        | 613      | ALLDPSFFAKESVKDAAGGPGAPADPGRPTGYSGSSKA                | none         | 3 (4)   | 1226.281 | 45.69                | 5.3   | 54.9   | x               | x                 | x               | 5  |
| 766 | 576        | 617      | ALLDPSFFAKESVKDAAGGPGAPADPGRPTGYSGSSKALVST            | none         | 4       | 1020.021 | 48.33                | 4.1   | 31.9   | x               | x                 | x               |  |
| 767 | 576        | 622      | ALLDPSFFAKESVKDAAGGPGAPADPGRPTGYSGSSKALVST<br>LVPLA   | none         | 4 (3)   | 1143.353 | 59.10                | 3.9   | 29.9   | x               | x                 | x               |  |
| 768 | 582        | 613      | FAKESVKDAAGGPGAPADPGRPTGYSGSSKA                       | none         | 4 (3,5) | 770.881  | 28.49                | 3.9   | 62.4   | x               | x                 | x               | 3; 5   |
| 769 | 583        | 613      | FAKESVKDAAGGPGAPADPGRPTGYSGSSKA                       | none         | 4 (3)   | 734.112  | 24.09                | 4.6   | 59.5   | x               | x                 | x               | 3  |
| 770 | 587        | 605      | SVKDAAGGPGAPADPGRPT                                   | none         | 3       | 574.291  | 19.15                | 3.8   | 64.9   |                 |                   | x               |  |
| 771 | 587        | 610      | SVKDAAGGPGAPADPGRPTGYSGS                              | none         | 3       | 724.682  | 22.81                | 4.1   | 59.2   |                 |                   | x               |  |
| 772 | 590        | 605      | DAAGGPGAPADPGRPT                                      | none         | 2       | 703.836  | 19.04                | 3.0   | 70.2   |                 |                   | x               |  |
| 773 | 590        | 622      | DAAGGPGAPADPGRPTGYSGSSKALVSTLVPLA                     | none         | 3       | 1013.193 | 50.88                | 3.0   | 44.0   | x               | x                 | x               |  |
| 774 | 591        | 605      | AAGGPGAPADPGRPT                                       | none         | 2       | 646.322  | 17.50                | 2.6   | 60.8   |                 |                   | x               |  |
| 775 | 591        | 613      | AAGGPGAPADPGRPTGYSGSSKA                               | none         | 3       | 676.995  | 20.62                | 1.8   | 32.4   | x               | x                 | x               |  |
| 776 | 601        | 614      | PGRPTGYSGSSKAL  | none         | 3       | 459.908  | 19.31                | 4.2   | 71.3   |                 | x                 | x               |  |
| 777 | 601        | 622      | PGRPTGYSGSSKALVSTLVPLA                                | none         | 3       | 720.067  | 47.96                | 1.5   | 39.5   | x               | x                 | x               |  |

Protein canopy homolog 3 (Q0P5N1)

| Nr.   | Start pos. | End pos. | Sequence                     | Modification | z       | m/z     | t <sub>r</sub> (min) | Xcorr | -10lgP | RM <sup>a</sup> | UH T <sup>a</sup> | IF <sup>a</sup> | Literature (milk <sup>1-6</sup> , colostrum <sup>7</sup> ) |
|---|------------|----------|------------------------------|--------------|---------|---------|----------------------|-------|--------|-----------------|-------------------|-----------------|--|
| 778   | 31         | 41       | LPAPELGPRQA                  | none         | 2       | 574.823 | 30.01                | 2.6   | 55.2   | x               | x                 | x               |  |
| <b>Protein OS-9 (Q3MHX6)</b>                                    |            |          |                              |              |         |         |                      |       |        |                 |                   |                 |  |
| 779   | 3          | 16       | VGSLNLEELSEMRY               | none         | 2       | 820.406 | 53.49                | 3.0   | 58.0   |                 |                   | x               |  |
| <b>Ribonuclease pancreatic (P61823)</b>                         |            |          |                              |              |         |         |                      |       |        |                 |                   |                 |  |
| 780   | 114        | 124      | PYVPVHFDASV                  | none         | 2       | 615.811 | 43.25                | 2.7   | 71.7   | x               | x                 |                 |  |
| <b>Secretoglobin family 1D member (A0JNP2)</b>                  |            |          |                              |              |         |         |                      |       |        |                 |                   |                 |  |
| 781   | 72         | 81       | VKAVLNPSSA                   | none         | 2       | 493.287 | 22.60                | 2.3   | 42.5   |                 | x                 |                 |  |
| <b>Serum albumin (P02769)</b>                                   |            |          |                              |              |         |         |                      |       |        |                 |                   |                 |  |
| 782   | 408        | 415      | FQNALIVR                     | none         | 2       | 480.785 | 33.47                | 2.3   | 43.3   | x               |                   |                 |  |
| 783   | 419        | 433      | KVPQVSTPTLVEVSR              | none         | 3 (2)   | 547.317 | 35.69                | 4.3   | 72.5   | x               |                   |                 |  |
| 784   | 99         | 112      | DPNHFRPAGLPDKY               | none         | 3       | 542.938 | 31.70                | 3.1   | 45.9   | x               | x                 |                 |  |
| <b>Sodium-dependent phosphate transport protein 2B (Q27960)</b> |            |          |                              |              |         |         |                      |       |        |                 |                   |                 |  |
| 785   | 3          | 26       | PWPELENSQPTSEKYTVKADGEQS     | none         | 3       | 907.428 | 37.29                | 3.0   | 55.0   | x               | x                 |                 |  |
| 786   | 4          | 16       | WPELENSQPTSEK                | none         | 2       | 772.866 | 33.22                | 3.4   | 63.6   | x               | x                 | x               |  |
| 787   | 4          | 25       | WPELENSQPTSEKYTVKADGEQ       | none         | 3       | 846.067 | 36.08                | 3.9   | 56.8   | x               | x                 | x               |  |
| 788   | 4          | 26       | WPELENSQPTSEKYTVKADGEQS      | none         | 3       | 875.076 | 35.82                | 5.2   | 68.4   | x               | x                 | x               |  |
| 789   | 6          | 26       | ELENSQPTSEKYTVKADGEQS        | none         | 3       | 780.700 | 23.64                | 3.1   | 34.6   | x               | x                 | x               |  |
| 790   | 26         | 53       | SAKPEAKETEKDDTGTPITKIELVPSH  | none         | 4 (5)   | 763.158 | 30.78                | 5.2   | 52.7   | x               | x                 | x               |  |
| 791   | 27         | 53       | AKPEAKETEKDDTGTPITKIELVPSH   | none         | 3 (4,5) | 988.201 | 30.74                | 4.8   | 60.1   | x               | x                 | x               |  |
| 792   | 31         | 53       | KAKETEKDDTGTPITKIELVPSH      | none         | 4       | 635.090 | 32.21                | 5.3   | 57.7   | x               | x                 | x               |  |
| 793   | 39         | 47       | DTGTPITKI                    | none         | 2       | 473.265 | 29.26                | 2.2   | 50.3   | x               | x                 | x               |  |
| 794   | 42         | 53       | TPITKIELVPSH                 | none         | 3       | 445.594 | 35.58                | 3.6   | 62.2   | x               | x                 | x               |  |
| 795   | 666        | 693      | MDKEAQDGVTKSEVDASGTKIVSSVTAL | none         | 3       | 956.151 | 44.54                | 5.0   | 51.1   | x               | x                 | x               |  |
| 796   | 666        | 693      | mDKEAQDGVTKSEVDASGTKIVSSVTAL | M1(Ox)       | 3       | 961.483 | 44.03                | 4.0   | 54.0   | x               |                   | x               |  |
| 797   | 667        | 683      | DKEAQDGVTKSEVDASG            | none         | 2       | 868.401 | 17.60                | 2.5   | 52.0   | x               |                   | x               |  |
| 798   | 667        | 685      | DKEAQDGVTKSEVDASGTK          | none         | 3       | 655.651 | 16.50                | 2.3   | 36.5   | x               |                   | x               |  |
| 799   | 667        | 693      | DKEAQDGVTKSEVDASGTKIVSSVTAL  | none         | 3       | 912.470 | 44.67                | 4.9   | 50.8   | x               | x                 | x               |  |
| <b>Syndecan-2 (Q58DD4)</b>                                      |            |          |                              |              |         |         |                      |       |        |                 |                   |                 |  |
| 800   | 99         | 120      | KTDPAEEDTNVYTEKHSDNLFK       | none         | 4       | 646.055 | 29.65                | 4.5   | 33.4   | x               | x                 |                 |  |

| Nr.  | Start pos. | End pos. | Sequence      | Modification | z | m/z     | t <sub>r</sub> (min) | Xcorr | -10lgP | RM <sup>a</sup> | UH T <sup>a</sup> | IF <sup>a</sup> | Literature (milk <sup>1-6</sup> , colostrum <sup>7</sup> ) |
|--|------------|----------|---------------|--------------|---|---------|----------------------|-------|--------|-----------------|-------------------|-----------------|--|
| <b>Xanthine dehydrogenase/oxidase (P80457)</b> |            |          |               |              |   |         |                      |       |        |                 |                   |                 |  |
| 801  | 563        | 575      | PNGQsKEDTVGRP | S5(Phospho)  | 2 | 732.827 | 15.44                | 2.5   | 32.1   | x               | x                 |                 |  |

\*Phosphorylation sites rely on sequences suggested by Proteome Discoverer 2.2 and PEAKS.

<sup>a</sup> It should be noted that the acquired LC-MS/MS data sets for the different milk types were not statistically different in terms of number of tandem mass spectra acquired per replicate (ranging from 2359 to 2735, with an average of 2541). Additionally, the overall peak area sum (sum of peak areas of all peptides in a sample replicate) was not significantly different between the samples ( $p > 0.09$ ).

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**Table S3:** Modified peptides identified by Proteome Discoverer 2.2 and manual confirmation of the modification sites. If the modified peptide was additionally proposed by PEAKS Studio 10.5, the “-10lgP” value is listed. An “x” indicates that the peptides was present in RM, UHT milk or IF, whereas a “blank” indicates that it was not detected.

| Nr.                             | Start pos. | End pos. | Mod. Site | Annotated Sequence      | Modifications      | z     | m/z     | tr (min) | XCorr | -10lgP | UH RM | T | IF |
|---------------------------------|------------|----------|-----------|-------------------------|--------------------|-------|---------|----------|-------|--------|-------|---|----|
| <b>Alpha-S1-casein (P02662)</b> |            |          |           |                         |                    |       |         |          |       |        |       |   |    |
| 1                               | 1          | 13       | K7        | RPKHPIkHQGLPQ           | K7(Lac)            | 4     | 465.754 | 13.13    | 1.8   |        |       | x |    |
| 2                               | 1          | 16       | K7        | RPKHPIkHQGLPQEVL        | K7(Lac)            | 4     | 551.053 | 22.65    | 3.0   | 18.8   |       | x |    |
| 3                               | 1          | 20       | K7        | RPKHPIkHQGLPQEVLNENL    | K7(Lac)            | 5     | 535.087 | 31.77    | 2.8   |        | x     | x |    |
| 4                               | 1          | 21       | K3        | RPkHPIKHQGLPQEVLNENLL   | K3(Lac)            | 5     | 557.704 | 37.90    | 2.3   | 27.1   | x     | x | x  |
| 5                               | 1          | 22       | K3        | RPkHPIKHQGLPQEVLNENLLR  | K3(Lac)            | 4     | 735.904 | 34.36    | 2.2   | 29.1   | x     | x | x  |
| 6                               | 1          | 22       | K3, K7    | RPkHPIkHQGLPQEVLNENLLR  | K3(Lac); K7(Lac)   | 5     | 653.747 | 34.04    | 4.8   | 28.0   |       |   | x  |
| 7                               | 1          | 22       | K7        | RPKHPIkHQGLPQEVLNENLLR  | K7(Lac)            | 5     | 588.926 | 34.43    | 5.4   | 13.9   | x     | x | x  |
| 8                               | 1          | 23       | K3        | RPkHPIKHQGLPQEVLNENLLRF | K3(Lac)            | 5 (4) | 618.339 | 44.04    | 5.0   | 28.0   | x     | x | x  |
| 9                               | 1          | 23       | K3, K7    | RPkHPIkHQGLPQEVLNENLLRF | K3(Lac); K7(Lac)   | 5     | 683.161 | 43.40    | 4.1   |        |       |   | x  |
| 10                              | 1          | 23       | K7        | RPKHPIkHQGLPQEVLNENLLRF | K7(Lac)            | 5     | 618.339 | 44.17    | 4.4   |        |       |   | x  |
| 11                              | 23         | 36       | K36       | FFVAPFPEVFGKEk          | K14(Lac)           | 3     | 655.999 | 53.52    | 2.5   | 28.2   | x     | x |    |
| 12                              | 23         | 37       | K36       | FFVAPFPEVFGKEkV         | K14(Lac)           | 3     | 689.020 | 55.98    | 3.0   | 37.2   |       |   | x  |
| 13                              | 23         | 42       | K36       | FFVAPFPEVFGKEkVNELSK    | K14(Lac)           | 4     | 659.842 | 52.29    | 4.0   | 37.7   |       |   | x  |
| 14                              | 24         | 36       | K36       | FVAPFPEVFGKEk           | K13(Hex)           | 3     | 552.956 | 47.39    | 2.8   | 28.0   |       |   | x  |
| 15                              | 24         | 38       | K34       | FVAPFPEVFGkEKVN         | K11(Lac)           | 3     | 678.012 | 47.61    | 3.2   |        |       |   | x  |
| 16                              | 24         | 39       | K34       | FVAPFPEVFGkEKVNNE       | K11(Lac)           | 3     | 721.026 | 47.67    | 2.5   | 21.6   |       |   | x  |
| 17                              | 24         | 41       | K36       | FVAPFPEVFGKEkVNELS      | K13(Hex)           | 3     | 733.715 | 51.70    | 2.6   |        |       |   | x  |
| 18                              | 24         | 42       | K34, K36  | FVAPFPEVFGkEkVNELSK     | K11(Hex); K13(Lac) | 4     | 663.588 | 46.51    | 3.6   | 24.3   |       |   | x  |
| 19                              | 24         | 42       | K34, K36  | FVAPFPEVFGkEkVNELSK     | K11(Lac); K13(Lac) | 4     | 704.101 | 46.31    | 3.5   | 39.6   |       |   | x  |
| 20                              | 24         | 42       | K36       | FVAPFPEVFGKEkVNELSK     | K13(Lac)           | 4     | 623.073 | 46.72    | 4.6   | 63.4   |       |   | x  |
| 21                              | 24         | 42       | K36       | FVAPFPEVFGKEkVNELSK     | K13(Hex)           | 4     | 582.561 | 47.19    | 5.6   | 53.5   |       |   | x  |
| 22                              | 25         | 36       | K34       | VAPFPEVFGkEK            | K10(Lac)           | 3     | 557.952 | 38.25    | 1.6   | 32.2   | x     | x |    |
| 23                              | 25         | 36       | K34       | VAPFPEVFGkEK            | K10(Hex)           | 3     | 503.932 | 39.07    | 1.8   | 9.0    |       |   | x  |
| 24                              | 25         | 37       | K34, K36  | VAPFPEVFGkEKV           | K10(Hex); K12(Lac) | 3     | 644.993 | 42.19    | 2.8   |        |       |   | x  |
| 25                              | 25         | 40       | K34       | VAPFPEVFGkEKVNEL        | K10(Lac)           | 3     | 709.699 | 47.30    | 2.7   |        |       |   | x  |

| Nr. | Start pos. | End pos. | Mod. Site  | Annotated Sequence        | Modifications                  | z     | m/z     | tr (min) | XCorr | -10lgP | RM | UH T | IF |
|-----|------------|----------|------------|---------------------------|--------------------------------|-------|---------|----------|-------|--------|----|------|----|
| 26  | 25         | 42       | K34        | VAPFPEVFGkEKVNELSK        | K10(Lac)                       | 4     | 586.308 | 40.86    | 4.1   | 49.4   |    | x    |    |
| 27  | 25         | 42       | K36        | VAPFPEVFGKEkVNELSK        | K12(Lac)                       | 4     | 586.307 | 41.01    | 3.5   | 63.0   |    | x    |    |
| 28  | 26         | 36       | K34        | APFPEVFGkEK               | K9(Lac)                        | 3     | 524.926 | 35.37    | 2.0   | 26.2   | x  | x    |    |
| 29  | 26         | 37       | K34        | APFPEVFGkEKV              | K9(Hex)                        | 3     | 503.933 | 40.21    | 2.4   | 29.6   |    | x    |    |
| 30  | 26         | 37       | K34, K36   | APFPEVFGkEkV              | K9(Lac); K11(Lac)              | 3     | 665.987 | 39.25    | 2.3   | 33.0   |    | x    |    |
| 31  | 28         | 37       | K34        | FPEVFGkEKV                | K7(Lac)                        | 3     | 501.920 | 35.84    | 2.5   | 27.1   |    | x    |    |
| 32  | 80         | 90       | K83        | HIQkEDVPSER               | K4(Lac)                        | 3     | 554.600 | 13.76    | 2.8   | 12.5   | x  | x    | x  |
| 33  | 80         | 91       | K83        | HIQkEDVPSERY              | K4(Lac)                        | 3     | 608.955 | 18.73    | 2.7   | 29.5   |    | x    | x  |
| 34  | 80         | 92       | K83        | HIQkEDVPSERYL             | K4(Lac)                        | 3     | 646.650 | 26.26    | 3.0   | 30.7   |    | x    |    |
| 35  | 80         | 93       | K83        | HIQkEDVPSERYLG            | K4(Lac)                        | 3     | 665.658 | 24.37    | 3.5   | 32.8   | x  | x    |    |
| 36  | 80         | 94       | K83        | HIQkEDVPSERYLGY           | K4(Lac)                        | 3     | 720.013 | 29.80    | 2.6   | 23.3   |    | x    |    |
| 37  | 80         | 96       | K83        | HIQkEDVPSERYLGYLE         | K4(Lac)                        | 3     | 800.722 | 37.83    | 1.9   | 10.9   |    | x    |    |
| 38  | 80         | 99       | K83        | HIQkEDVPSERYLGYLEQLL      | K4(Lac)                        | 4     | 689.349 | 60.43    | 2.5   | 17.4   | x  | x    |    |
| 39  | 80         | 100      | K83        | HIQkEDVPSERYLGYLEQLLR     | K4(Lac)                        | 4     | 728.376 | 57.22    | 5.1   | 51.1   | x  | x    |    |
| 40  | 80         | 100      | K83        | HIQkEDVPSERYLGYLEQLLR     | K4(Hex)                        | 4     | 687.862 | 57.64    | 5.2   | 51.7   |    | x    |    |
| 41  | 80         | 101      | K83        | HIQkEDVPSERYLGYLEQLLRL    | K4(Lac)                        | 4     | 756.649 | 66.16    | 5.1   | 36.8   | x  | x    |    |
| 42  | 80         | 102      | K102       | HIQKEDVPSERYLGYLEQLLRLK   | K23(Lac)                       | 5 (4) | 631.136 | 59.33    | 6.7   | 42.8   | x  | x    | x  |
| 43  | 80         | 102      | K83        | HIQkEDVPSERYLGYLEQLLRLK   | K4(Lac)                        | 5     | 631.138 | 60.64    | 5.0   | 26.9   | x  | x    | x  |
| 44  | 80         | 102      | K83        | HIQkEDVPSERYLGYLEQLLRLK   | K4(Hex)                        | 5     | 598.726 | 60.17    | 6.5   | 36.4   |    | x    |    |
| 45  | 80         | 102      | K83, K102  | HIQkEDVPSERYLGYLEQLLRLK   | K4(Lac); K23(Lac)              | 5     | 695.959 | 58.72    | 5.8   |        |    | x    |    |
| 46  | 80         | 103      | K102       | HIQKEDVPSERYLGYLEQLLRLKK  | K23(Lac)                       | 5     | 656.758 | 55.15    | 4.7   | 29.5   | x  | x    |    |
| 47  | 80         | 104      | K102       | HIQKEDVPSERYLGYLEQLLRLKKY | K23(Lac)                       | 5     | 689.369 | 55.84    | 4.5   | 25.9   | x  | x    |    |
| 48  | 80         | 104      | K103       | HIQKEDVPSERYLGYLEQLLRLKKY | K24(Lac)                       | 5     | 689.370 | 55.89    | 4.8   | 30.6   |    | x    |    |
| 49  | 81         | 90       | K83        | IQkEDVPSE                 | K3(Lac)                        | 3     | 508.914 | 14.69    | 2.6   | 15.1   | x  | x    |    |
| 50  | 81         | 90       | K83        | IQkEDVPSE                 | K3(Hex)                        | 3     | 454.896 | 15.28    | 2.0   |        |    | x    |    |
| 51  | 81         | 91       | K83        | QkEDVPSE                  | K2(Lac)                        | 3     | 525.573 | 17.67    | 1.6   | 12.2   | x  | x    |    |
| 52* | 103        | 123      | K103       | kYKVPQLEIVPNsAEERLHSM     | K1(Lac); S13(Phospho)          | 4     | 718.849 | 44.17    | 4.0   |        | x  | x    | x  |
| 53* | 103        | 123      | K103       | kYKVPQLEIVPNsAEERLHSm     | K1(Lac); S13(Phospho); M21(Ox) | 4     | 722.849 | 39.10    | 3.5   |        | x  | x    | x  |
| 54* | 103        | 123      | K103, K105 | kYkVPQLEIVPNsAEERLHSM     | K1(Hex); K3(Hex); S13(Phospho) | 4     | 718.850 | 44.18    | 3.9   |        | x  | x    | x  |

| Nr.                             | Start pos. | End pos. | Mod. Site  | Annotated Sequence        | Modifications                           | z | m/z     | tr (min) | XCorr | -10lgP | RM | UH T | IF |
|---------------------------------|------------|----------|------------|---------------------------|---|---|---------|----------|-------|--------|----|------|----|
| 55*                             | 103        | 123      | K103, K105 | kYkVPQLEIVPNsAEERLHSm     | K1(Hex); K3(Hex); S13(Phospho); M21(Ox) | 4 | 722.849 | 38.99    | 3.7   |        |    | x    | x  |
| 56*                             | 103        | 123      | K103, K105 | kYkVPQLEIVPNsAEERLHSM     | K1(Lac); K3(Lac); S13(Phospho)          | 4 | 799.878 | 43.93    | 2.8   |        |    | x    |    |
| 57*                             | 103        | 123      | K105       | KYkVPQLEIVPNsAEERLHSm     | K3(Lac); S13(Phospho); M21(Ox)          | 4 | 722.849 | 39.06    | 3.5   | 45.4   |    | x    | x  |
| 58*                             | 103        | 123      | K105       | KYkVPQLEIVPNsAEERLHSM     | K3(Hex); S13(Phospho)                   | 4 | 678.337 | 44.31    | 4.2   | 39.3   |    | x    |    |
| 59*                             | 103        | 124      | K103, K105 | KYkVPQLEIVPNsAEERLHSMK    | K1(Hex); K3(Hex); S13(Phospho)          | 4 | 750.873 | 40.28    | 3.0   |        |    | x    | x  |
| 60*                             | 103        | 124      | K105       | KYkVPQLEIVPNsAEERLHSMK    | K3(Lac); S13(Phospho)                   | 4 | 750.872 | 40.47    | 2.4   |        |    | x    | x  |
| 61                              | 104        | 123      | K105       | YkVPQLEIVPNsAEERLHSM      | K2(Lac)                                 | 4 | 666.834 | 45.56    | 3.3   | 48.8   |    | x    | x  |
| 62*                             | 104        | 123      | K105       | YkVPQLEIVPNsAEERLHSM      | K2(Lac); S12(Phospho)                   | 4 | 686.826 | 47.74    | 3.2   | 36.2   |    | x    |    |
| 63*                             | 105        | 123      | K105       | kVPQLEIVPNsAEERLHSM       | K1(Lac); S11(Phospho)                   | 4 | 646.060 | 44.37    | 4.4   | 39.7   |    | x    |    |
| 64*                             | 105        | 124      | K105       | kVPQLEIVPNsAEERLHSMK      | K1(Lac); S11(Phospho)                   | 4 | 678.084 | 39.97    | 2.9   |        |    | x    |    |
| <b>Alpha-S2-casein (P02663)</b> |            |          |            |                           |   |   |         |          |       |        |    |      |    |
| 65                              | 1          | 24       | K21        | KNTMEHVSSSEESIIISQETYkQEK | K21(Lac)                                | 4 | 784.863 | 29.54    | 4.4   | 44.2   |    | x    | x  |
| 66*                             | 1          | 24       | K21        | KNTMEHVSSSEESIIIsQETYkQEK | S16(Phospho); K21(Lac)                  | 4 | 804.860 | 30.25    | 3.4   | 35.8   |    | x    | x  |
| 67                              | 1          | 24       | K24        | KNTMEHVSSSEESIIISQETYKQEK | K24(Lac)                                | 4 | 784.867 | 29.46    | 5.3   | 40.8   |    | x    | x  |
| 68                              | 1          | 24       | K24        | KNTmEHVSSSEESIIISQETYKQEK | M4(Ox); K24(Lac)                        | 4 | 788.865 | 26.08    | 3.2   |        |    | x    | x  |
| 69*                             | 1          | 24       | K24        | KNTmEHVSSSEESIIIsQETYKQEK | M4(Ox); S16(Phospho); K24(Lac)          | 4 | 808.858 | 26.96    | 3.2   |        |    | x    | x  |
| 70*                             | 1          | 24       | K24        | KNTMEHVSSSEEsIIISQETYKQEK | S13(Phospho); K24(Lac)                  | 4 | 804.861 | 30.38    | 3.2   | 19.6   |    | x    | x  |
| 71*                             | 137        | 150      | K150       | KTVDMEMsTEVFTKk           | S7(Phospho); K14(Lac)                   | 3 | 682.976 | 26.97    | 4.2   | 44.0   | x  | x    | x  |
| 72*                             | 138        | 150      | K150       | TVDMEMsTEVFTKk            | S6(Phospho); K13(Lac)                   | 3 | 640.278 | 30.53    | 2.0   | 21.6   |    | x    | x  |
| 73                              | 138        | 150      | K150       | TVDMESTEVFTKk             | K13(Lac)                                | 3 | 613.620 | 30.00    | 2.2   | 21.3   |    | x    | x  |
| 74                              | 150        | 162      | K150, K152 | kTKLTEEKNRLN              | K1(Lac); K3(Lac)                        | 4 | 563.528 | 14.36    | 2.9   | 22.2   |    | x    |    |
| 75                              | 150        | 163      | K150       | kTKLTEEKNRLNF             | K1(Lac)                                 | 4 | 519.269 | 24.23    | 5.5   | 57.5   |    | x    |    |
| 76                              | 150        | 163      | K150, K152 | kTKLTEEKNRLNF             | K1(Lac); K3(Lac)                        | 4 | 600.297 | 23.94    | 3.2   |        |    | x    |    |
| 77                              | 150        | 163      | K152       | kTKLTEEKNRLNF             | K3(Hex)                                 | 4 | 478.756 | 24.41    | 3.9   |        |    | x    |    |
| 78                              | 150        | 163      | K152       | kTKLTEEKNRLNF             | K3(Lac)                                 | 4 | 519.272 | 24.18    | 4.9   |        |    | x    |    |
| 79                              | 150        | 163      | K152, K158 | kTKLTEEENRLNF             | K3(Lac); K9(Lac)                        | 4 | 600.296 | 24.25    | 3.4   |        |    | x    |    |
| 80                              | 150        | 163      | K158       | KTKLTEEENRLNF             | K9(Lac)                                 | 3 | 692.026 | 24.31    | 3.0   |        |    | x    |    |
| 81                              | 150        | 164      | K150       | kTKLTEEKNRLNFL            | K1(Lac)                                 | 3 | 729.720 | 31.77    | 2.1   | 9.4    |    | x    | x  |
| 82                              | 150        | 164      | K150, K152 | kTKLTEEKNRLNFL            | K1(Lac); K3(Lac)                        | 4 | 628.569 | 31.48    | 3.4   |        |    | x    |    |

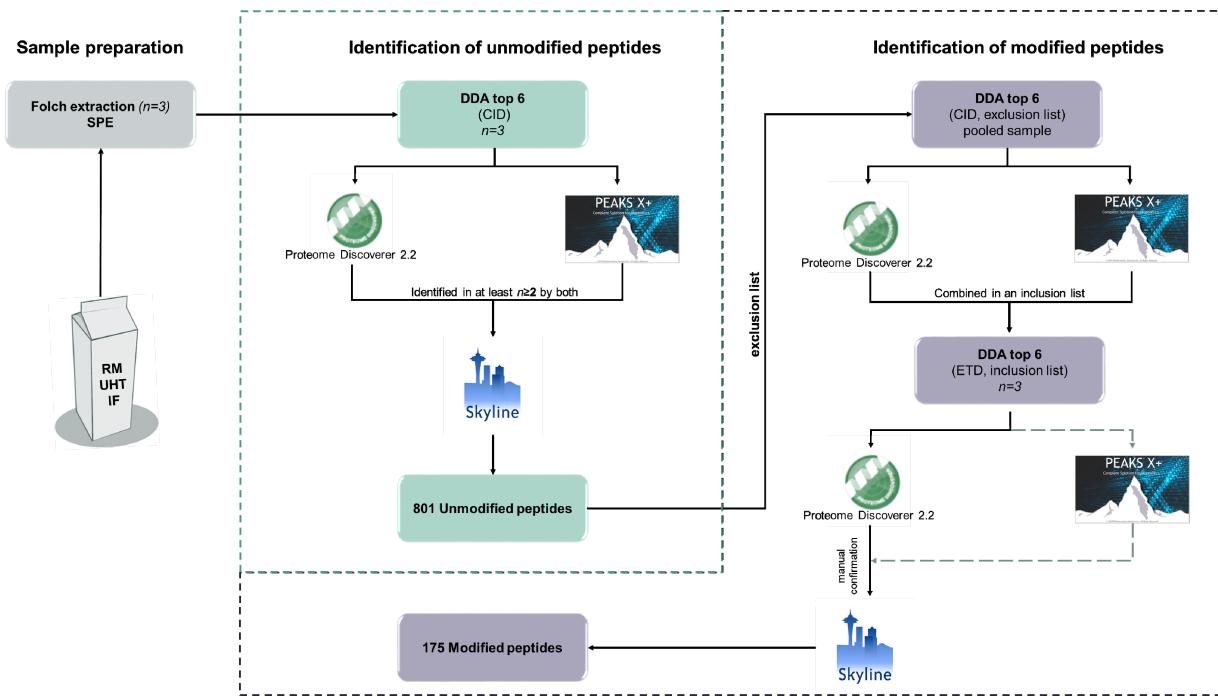
| Nr. | Start pos. | End pos. | Mod. Site  | Annotated Sequence  | Modifications     | z     | m/z     | tr (min) | XCorr | -10lgP | RM | UH T | IF |
|-----|------------|----------|------------|---------------------|-------------------|-------|---------|----------|-------|--------|----|------|----|
| 83  | 150        | 164      | K152       | KTkLTEEKNRLNFL      | K3(Hex)           | 4     | 507.027 | 32.14    | 4.1   | 43.7   |    | x    |    |
| 84  | 150        | 164      | K152       | KTKLTEEKNRLNFL      | K3(Lac)           | 4     | 547.542 | 31.69    | 4.1   | 48.6   | x  | x    | x  |
| 85  | 150        | 164      | K158       | KTKLTEEKNRLNFL      | K9(Lac)           | 4     | 547.540 | 31.96    | 4.8   | 36.4   | x  | x    | x  |
| 86  | 150        | 165      | K150       | KTKLTEEKNRLNFLK     | K1(Lac)           | 4 (5) | 579.566 | 27.33    | 5.6   | 42.7   | x  | x    | x  |
| 87  | 150        | 165      | K150, K152 | KTKLTEEKNRLNFLK     | K1(Lac); K3(Lac)  | 5     | 528.674 | 27.07    | 5.2   |        |    |      | x  |
| 88  | 150        | 165      | K152       | KTKLTEEKNRLNFLK     | K3(Lac)           | 5     | 463.852 | 27.56    | 5.9   | 34.9   | x  | x    |    |
| 89  | 150        | 165      | K152, K158 | KTKLTEEKNRLNFLK     | K3(Lac); K9(Lac)  | 5 (4) | 528.674 | 27.19    | 5.1   | 43.5   |    |      | x  |
| 90  | 150        | 165      | K158       | KTKLTEEKNRLNFLK     | K9(Lac)           | 5     | 463.853 | 27.36    | 5.6   | 31.8   | x  | x    | x  |
| 91  | 150        | 165      | K165       | KTKLTEEKNRLNFLk     | K16(Lac)          | 4     | 579.565 | 27.38    | 4.7   | 42.7   | x  | x    | x  |
| 92  | 151        | 161      | K152       | TkLTEEKNRL          | K2(Hex)           | 3     | 508.269 | 19.07    | 2.5   | 18.1   |    |      | x  |
| 93  | 151        | 161      | K152       | TkLTEEKNRL          | K2(Lac)           | 3     | 562.287 | 18.95    | 2.5   | 31.7   |    |      | x  |
| 94  | 151        | 161      | K152, K158 | TkLTEEKNRL          | K2(Lac); K8(Lac)  | 3     | 670.324 | 18.65    | 3.2   | 31.7   |    |      | x  |
| 95  | 151        | 161      | K158       | TKLTEEEKNRL         | K8(Lac)           | 3     | 562.288 | 18.63    | 3.1   | 32.6   |    |      | x  |
| 96  | 151        | 162      | K152, K158 | TkLTEEKNRLN         | K2(Lac); K8(Lac)  | 4     | 531.505 | 16.72    | 4.1   | 32.8   |    |      | x  |
| 97  | 151        | 162      | K158       | TKLTEEEKNRLN        | K8(Lac)           | 4 (3) | 450.478 | 16.55    | 4.6   | 40.7   | x  | x    |    |
| 98  | 151        | 162      | K158       | TKLTEEEKNRLN        | K8(Hex)           | 3     | 546.284 | 17.00    | 2.8   | 17.9   |    |      | x  |
| 99  | 151        | 163      | K152, K158 | TkLTEEKNRLNF        | K2(Lac); K8(Lac)  | 3     | 757.362 | 27.99    | 2.6   | 28.0   |    |      | x  |
| 100 | 151        | 163      | K158       | TKLTEEEKNRLNF       | K8(Lac)           | 3     | 649.325 | 28.38    | 3.7   | 26.2   |    |      | x  |
| 101 | 151        | 164      | K152       | TkLTEEEKNRLNFL      | K2(Lac)           | 3     | 687.022 | 35.78    | 3.3   | 35.9   | x  | x    |    |
| 102 | 151        | 164      | K158       | TKLTEEEKNRLNFL      | K8(Lac)           | 4 (3) | 515.517 | 36.11    | 5.0   | 33.6   | x  | x    |    |
| 103 | 151        | 164      | K158       | TKLTEEEKNRLNFL      | K8(Hex)           | 3     | 633.003 | 36.19    | 3.3   |        |    |      | x  |
| 104 | 151        | 165      | K152       | TKLTEEEKNRLNFLK     | K2(Lac)           | 3     | 729.719 | 31.10    | 2.5   | 29.4   | x  | x    |    |
| 105 | 151        | 165      | K158       | TKLTEEEKNRLNFLK     | K8(Lac)           | 4     | 547.541 | 31.09    | 5.0   | 59.9   | x  | x    | x  |
| 106 | 151        | 165      | K158       | TKLTEEEKNRLNFLK     | K8(Hex)           | 4     | 507.027 | 31.13    | 3.4   |        | x  | x    | x  |
| 107 | 151        | 165      | K158, K165 | TkLTEEEKNRLNFLk     | K8(Lac); K15(Lac) | 4     | 628.568 | 30.73    | 4.3   | 34.5   |    |      | x  |
| 108 | 151        | 165      | K165       | TKLTEEEKNRLNFLK     | K15(Lac)          | 4     | 547.540 | 30.68    | 4.6   | 40.9   | x  | x    | x  |
| 109 | 151        | 169      | K152       | TkLTEEEKNRLNFLKKISQ | K2(Lac)           | 4     | 661.610 | 35.50    | 4.0   |        | x  | x    | x  |
| 110 | 152        | 163      | K158       | KLTEEEKNRLNF        | K7(Lac)           | 3     | 615.643 | 26.00    | 2.9   |        |    |      | x  |
| 111 | 153        | 162      | K158       | LTEEEKNRLN          | K6(Lac)           | 3     | 523.922 | 14.31    | 2.6   | 13.4   |    |      | x  |
| 112 | 153        | 163      | K158       | LTEEEKNRLNF         | K6(Lac)           | 3     | 572.944 | 28.00    | 3.0   | 28.4   |    |      | x  |

| Nr.                         | Start pos. | End pos. | Mod. Site  | Annotated Sequence       | Modifications                  | z     | m/z     | tr (min) | XCorr | -10lgP | RM | UH T | IF |
|-----------------------------|------------|----------|------------|--------------------------|--------------------------------|-------|---------|----------|-------|--------|----|------|----|
| 113                         | 153        | 165      | K158       | LTEEEkNRLNFLK            | K6(Lac)                        | 3     | 653.336 | 31.23    | 1.9   | 9.8    |    | x    |    |
| 114                         | 153        | 165      | K158, K165 | LTEEEkNRLNFLk            | K6(Lac); K13(Lac)              | 4     | 571.282 | 30.55    | 4.3   |        |    | x    |    |
| 115                         | 154        | 163      | K158       | TEEEkNRLNF               | K5(Lac)                        | 3     | 535.251 | 23.49    | 2.6   |        |    | x    |    |
| 116                         | 154        | 164      | K158       | TEEEkNRLNFL              | K5(Lac)                        | 3     | 572.945 | 34.52    | 2.6   | 25.8   | x  | x    |    |
| 117                         | 154        | 165      | K158       | TEEEkNRLNFLK             | K5(Lac)                        | 4     | 461.984 | 26.98    | 4.5   | 34.3   |    | x    |    |
| 118                         | 155        | 163      | K158       | EEEkNRLNF                | K4(Lac)                        | 3     | 501.567 | 22.91    | 2.6   | 20.3   |    | x    |    |
| 119                         | 155        | 164      | K158       | EEEkNRLNFL               | K4(Lac)                        | 3     | 539.262 | 34.46    | 2.9   | 31.3   | x  | x    |    |
| 120                         | 170        | 179      | K173       | RYQkFALPQY               | K4(Lac)                        | 3     | 546.607 | 34.97    | 2.2   | 10.3   |    | x    |    |
| 121                         | 185        | 197      | K188       | QHQkAMkPWIQPK            | K4(Lac); K7(Lac)               | 4     | 567.781 | 19.03    | 3.2   | 18.8   |    | x    |    |
| 122*                        | 22         | 41       | T38        | QEKNmAINPsKENLCStFCK     | M5(Ox); S10(Phospho); T17(TOx) | 4     | 595.511 | 34.35    | 4.1   |        | x  | x    |    |
| 123                         | 22         | 41       | T38        | QEKNmAINPSKENLCStFCK     | M5(Ox); T17(TOx)               | 4     | 575.519 | 32.24    | 4.9   |        | x  | x    |    |
| 124*                        | 22         | 41       | T38        | QEKNMAINPsKENLCStFCK     | S10(Phospho); T17(TOx)         | 4     | 591.513 | 37.73    | 4.8   | 8.6    | x  | x    |    |
| 125                         | 22         | 41       | T38        | QEKNMAINPSKENLCStFCK     | T17(TOx)                       | 4     | 571.520 | 35.47    | 5.2   | 51.1   | x  | x    |    |
| 126*                        | 22         | 45       | T38        | QEKNmAINPsKENLCStFCKEVVR | M5(Ox); S10(Phospho); T17(TOx) | 4     | 716.332 | 40.23    | 4.9   |        | x  | x    |    |
| 127                         | 22         | 45       | T38        | QEKNmAINPSKENLCStFCKEVVR | M5(Ox); T17(TOx)               | 5     | 557.273 | 37.97    | 4.9   |        | x  | x    | x  |
| 128*                        | 22         | 45       | T38        | QEKNMAINPsKENLCStFCKEVVR | S10(Phospho); T17(TOx)         | 4     | 712.334 | 42.84    | 4.7   | 13.8   | x  | x    |    |
| 129                         | 22         | 45       | T38        | QEKNMAINPSKENLCStFCKEVVR | T17(TOx)                       | 4 (5) | 692.341 | 40.20    | 4.7   | 45.1   | x  | x    | x  |
| 130*                        | 25         | 41       | T38        | NmAINPsKENLCStFCK        | M2(Ox); S7(Phospho); T14(TOx)  | 3     | 665.283 | 37.32    | 3.0   |        | x  | x    | x  |
| 131                         | 25         | 41       | T38        | NmAINPSKENLCStFCK        | M2(Ox); T14(TOx)               | 3     | 638.625 | 34.94    | 3.5   |        | x  | x    | x  |
| 132*                        | 25         | 41       | T38        | NMAINPsKENLCStFCK        | S7(Phospho); T14(TOx)          | 3     | 659.949 | 41.81    | 2.5   |        | x  | x    | x  |
| 133                         | 25         | 41       | T38        | NMAINPSKENLCStFCK        | T14(TOx)                       | 3     | 633.294 | 39.11    | 2.9   | 24.6   | x  | x    | x  |
| 134*                        | 25         | 45       | T38        | NmAINPsKENLCStFCKEVVR    | M2(Ox); S7(Phospho); T14(TOx)  | 4     | 620.032 | 43.07    | 4.8   |        | x  | x    | x  |
| 135                         | 25         | 45       | T38        | NmAINPSKENLCStFCKEVVR    | M2(Ox); T14(TOx)               | 4     | 600.041 | 40.14    | 4.3   |        | x  | x    | x  |
| 136*                        | 25         | 45       | T38        | NMAINPsKENLCStFCKEVVR    | S7(Phospho); T14(TOx)          | 4     | 616.034 | 46.37    | 4.4   |        | x  | x    | x  |
| 137                         | 25         | 45       | T38        | NMAINPSKENLCStFCKEVVR    | T14(TOx)                       | 4     | 596.043 | 43.35    | 4.8   | 45.1   | x  | x    | x  |
| <b>Beta-casein (P02666)</b> |            |          |            |                          |                                |       |         |          |       |        |    |      |    |
| 138*                        | 29         | 40       | K29        | KIEKFQsEEQQQ             | K1(Lac); S7(Phospho)           | 3     | 642.614 | 17.96    | 2.1   | 11.4   |    | x    |    |
| 139                         | 29         | 48       | K29        | KIEKFQSEEQQQTDELQDK      | K1(Lac)                        | 4     | 701.828 | 25.70    | 3.2   | 34.3   | x  | x    |    |
| 140*                        | 29         | 48       | K29        | KIEKFQsEEQQQTDELQDK      | K1(Lac); S7(Phospho)           | 4     | 721.820 | 28.68    | 4.5   |        | x  | x    |    |
| 141                         | 29         | 48       | K32        | KIEkFQSEEQQQTDELQDK      | K4(Lac)                        | 4     | 701.829 | 26.21    | 4.5   | 52.7   | x  | x    | x  |

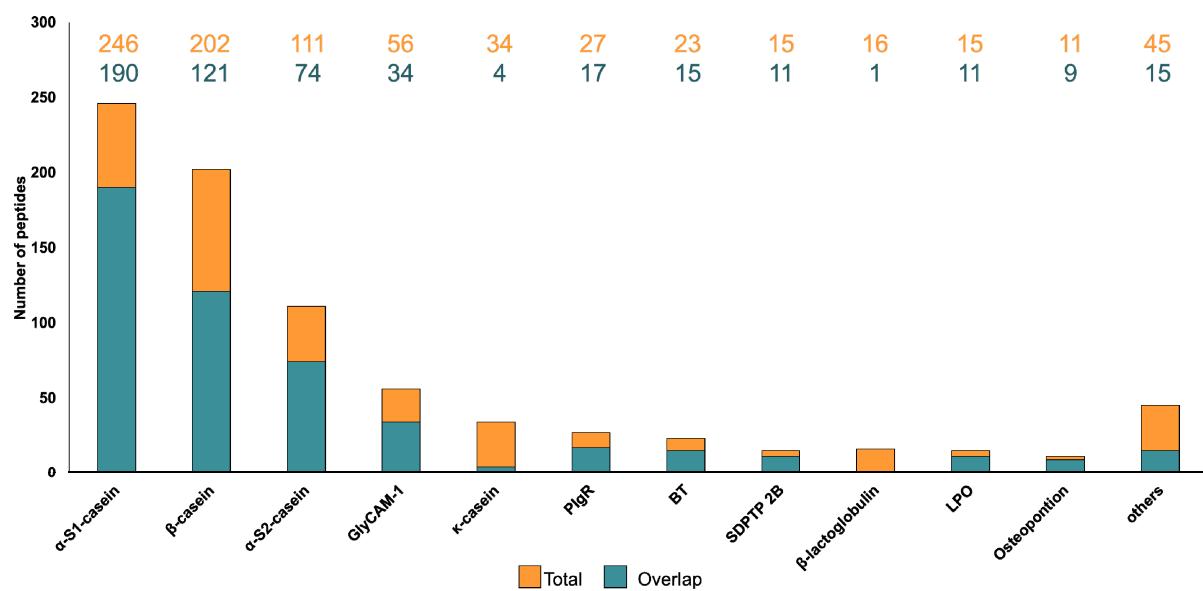
| Nr.  | Start pos. | End pos. | Mod. Site  | Annotated Sequence         | Modifications        | z     | m/z     | tr (min) | XCorr | -10lgP | RM | UH T | IF |
|--|------------|----------|------------|----------------------------|----------------------|-------|---------|----------|-------|--------|----|------|----|
| 142*   | 29         | 48       | K32        | KIEkFQsEEQQQTEDELQDK       | K4(Lac); S7(Phospho) | 4     | 721.820 | 28.48    | 4.4   | 42.7   | x  | x    | x  |
| <b>Butyrophilin subfamily 1 member A1 (P18892)</b>               |            |          |            |                            |                      |       |         |          |       |        |    |      |    |
| 143  | 153        | 177      | P160       | THRGEFPMSERSNPDEEGLFTVR    | P8(Ox)               | 5     | 585.472 | 34.45    | 5.0   | 32.8   | x  | x    | x  |
| <b>Fibroblast growth factor-binding protein 1 (Q9MZ06)</b>       |            |          |            |                            |                      |       |         |          |       |        |    |      |    |
| 144  | 6          | 27       | K22        | NRRGSKASADESALGkPGKEPR     | K17(Lac)             | 5 (6) | 550.488 | 17.22    | 3.8   | 13.2   | x  | x    | x  |
| 145  | 8          | 27       | K25        | RGSKASADESALGKPGkEPR       | K18(Lac)             | 5     | 496.459 | 18.43    | 5.8   | 24.0   | x  | x    | x  |
| 146  | 9          | 27       | K22        | GSKASADESALGkPGKEPR        | K14(Lac)             | 5 (4) | 465.239 | 20.15    | 4.7   | 39.3   | x  | x    | x  |
| 147  | 9          | 27       | K25        | GSKASADESALGKPGkEPR        | K17(Lac)             | 4     | 581.298 | 20.10    | 3.6   | x      | x  | x    | x  |
| <b>Glycosylation-dependent cell adhesion molecule 1 (P80195)</b> |            |          |            |                            |                      |       |         |          |       |        |    |      |    |
| 148  | 1          | 10       | K4         | ILNkPEDETH                 | K4(Lac)              | 3     | 507.238 | 14.06    | 1.9   | 9.2    | x  |      |    |
| 149  | 1          | 11       | K4         | ILNkPEDETHL                | K4(Lac)              | 3     | 544.933 | 24.44    | 2.3   | 34.2   | x  |      |    |
| 150  | 1          | 12       | K4         | ILNkPEDETHLE               | K4(Lac)              | 3     | 587.948 | 23.42    | 3.0   | 32.3   | x  |      |    |
| 151  | 1          | 16       | K4         | ILNkPEDETHLEAQPT           | K4(Lac)              | 3     | 720.350 | 25.40    | 2.7   | 27.0   | x  |      |    |
| 152  | 1          | 24       | K4         | ILNkPEDETHLEAQPTDASAQFIR   | K4(Lac)              | 4     | 762.630 | 35.75    | 5.4   | 59.0   | x  | x    | x  |
| 153  | 1          | 26       | K4         | ILNkPEDETHLEAQPTDASAQFIRNL | K4(Lac)              | 4     | 819.408 | 46.22    | 3.9   | 33.3   | x  |      |    |
| 154  | 2          | 13       | K4         | LNkPEDETHLE                | K3(Lac)              | 3     | 550.253 | 19.98    | 2.4   | 30.5   | x  |      |    |
| 155  | 54         | 67       | K64        | SSRQPQSQNPKLPL             | K11(Hex)             | 3     | 581.308 | 27.54    | 2.0   | 16.1   | x  |      |    |
| 156  | 54         | 70       | K64        | SSRQPQSQNPKLPLSIL          | K11(Hex)             | 3     | 685.710 | 44.63    | 3.8   | 10.1   | x  |      |    |
| 157  | 54         | 71       | K71        | SSRQPQSQNPKLPLSILk         | K18(Lac)             | 4     | 587.071 | 36.31    | 4.5   | 41.3   | x  |      |    |
| 158  | 54         | 73       | K71        | SSRQPQSQNPKLPLSILkEK       | K18(Lac)             | 5 (4) | 521.285 | 33.40    | 3.7   | 10.0   | x  | x    |    |
| 159  | 54         | 73       | K71, K73   | SSRQPQSQNPKLPLSILkEk       | K18(Lac); K20(Lac)   | 5     | 586.107 | 32.73    | 4.8   |        | x  |      |    |
| 160  | 54         | 73       | K73        | SSRQPQSQNPKLPLSILKEk       | K20(Lac)             | 5 (4) | 521.285 | 33.30    | 4.9   | 31.7   | x  | x    |    |
| 161  | 54         | 75       | K64, K73   | SSRQPQSQNPKLPLSILkEKHL     | K11(Lac); K18(Lac)   | 5     | 636.134 | 35.60    | 3.1   |        | x  |      |    |
| 162  | 54         | 75       | K71        | SSRQPQSQNPKLPLSILkEKHL     | K18(Lac)             | 5     | 571.314 | 35.94    | 6.1   | 47.2   | x  |      |    |
| 163  | 54         | 75       | K73        | SSRQPQSQNPKLPLSILKEkHL     | K20(Lac)             | 5 (4) | 571.315 | 35.40    | 6.4   | 37.2   | x  |      |    |
| 164  | 109        | 121      | K116, K120 | RNLENTVketikY              | K8(Lac); K12(Lac)    | 3     | 752.702 | 32.21    | 3.0   | 22.6   | x  |      |    |
| 165  | 109        | 121      | K120       | RNLENTVketikY              | K12(Lac)             | 3     | 644.665 | 32.31    | 3.8   | 42.7   | x  |      |    |
| 166  | 111        | 121      | K116, K120 | LENTVketikY                | K6(Lac); K10(Lac)    | 3     | 662.653 | 26.84    | 2.0   | 17.9   | x  |      |    |
| 167  | 111        | 121      | K120       | LENTVKETIKY                | K10(Lac)             | 3     | 554.618 | 27.24    | 2.8   |        | x  |      |    |
| 168  | 112        | 121      | K116       | ENTVketikY                 | K5(Lac)              | 3     | 516.923 | 22.96    | 3.1   | 35.0   | x  |      |    |

| Nr.                             | Start pos. | End pos. | Mod. Site  | Annotated Sequence | Modifications    | z | m/z     | tr (min) | XCorr | -10lgP | RM | UH T | IF |
|---------------------------------|------------|----------|------------|--------------------|------------------|---|---------|----------|-------|--------|----|------|----|
| 169                             | 112        | 121      | K116, K120 | ENTVkETIkY         | K5(Lac); K9(Lac) | 3 | 624.958 | 22.73    | 2.1   | 24.9   |    | x    |    |
| 170                             | 123        | 135      | K134       | KSLFSHAFEVVkT      | K12(Lac)         | 3 | 606.313 | 38.11    | 2.6   |        |    | x    |    |
| 171                             | 126        | 135      | K134       | FSHAFEVVKT         | K9(Lac)          | 3 | 496.909 | 29.14    | 2.8   | 41.3   |    | x    |    |
| 172                             | 126        | 135      | K134       | FSHAFEVVKT         | K9(Hex)          | 3 | 442.891 | 29.73    | 2.4   | 43.6   |    | x    |    |
| 173                             | 127        | 135      | K134       | SHAFEVVKT          | K8(Lac)          | 3 | 447.886 | 21.75    | 2.1   |        |    | x    |    |
| <b>Lactoperoxidase (P80025)</b> |            |          |            |                    |                  |   |         |          |       |        |    |      |    |
| 174                             | 68         | 76       | K74        | VWEESLkRL          | K7(Lac)          | 3 | 495.255 | 34.81    | 2.1   | 27.2   | x  | x    |    |
| 175                             | 69         | 76       | K74        | WEESLkRL           | K6(Lac)          | 3 | 462.233 | 30.59    | 2.1   | 13.1   |    | x    |    |

\*Phosphorylation sites rely on software tools without further confirmation of their location.



**Figure S1:** Strategy applied for the identification of unmodified and modified endogenous peptides in RM, UHT milk, and IF relying on software tools Proteome Discoverer 2.2 and PEAKS 10.5 in combination with a spectra library generated within Skyline.



**Figure S2:** Total number of peptides identified for different proteins (orange) and the number of overlapping peptides (blue) present in RM, UHT milk, and IF. Abbreviations: GlyCAM-1 - glycosylation-dependent cell adhesion molecule 1, PigR - polymeric immunoglobulin receptor, BT - butyrophilin subfamily 1 member A1, SDPTP 2B - sodium-dependent phosphate transport protein 2B, and LPO – lactoperoxidase.

| Position | 1   | 2   | 3   | 4   | 5   | 6   | 7   | 8   | 9   | 10  | 11  | 12  | 13  | 14  | 15  | 16  | 17  | 18  | 19  | 20  | 21  | 22  | 23  | 24  | 25  | 26  | 27  | 28  | 29    | 30    | Position |       |    |    |     |
|----------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-------|-------|----------|-------|----|----|-----|
| AA       | R   | P   | K   | H   | P   | I   | K   | H   | Q   | G   | L   | P   | Q   | E   | V   | L   | N   | E   | N   | L   | R   | F   | V   | A   | P   | F   | P   | E   | AA    |       |          |       |    |    |     |
| Total    | 2   | 2   | 2   | 6   | 6   | 6   | 8   | 10  | 14  | 21  | 25  | 25  | 27  | 31  | 33  | 36  | 37  | 35  | 34  | 33  | 31  | 24  | 22  | 18  | 22  | 30  | 33  | 36  | 36    | Total |          |       |    |    |     |
| RM       | 2   | 2   | 2   | 6   | 6   | 6   | 7   | 9   | 10  | 15  | 19  | 19  | 20  | 22  | 24  | 27  | 28  | 27  | 27  | 26  | 24  | 19  | 17  | 17  | 22  | 30  | 33  | 36  | 36    | RM    |          |       |    |    |     |
| UHT      | 2   | 2   | 2   | 6   | 6   | 6   | 7   | 9   | 10  | 15  | 19  | 19  | 20  | 22  | 24  | 27  | 28  | 27  | 27  | 26  | 24  | 19  | 17  | 17  | 22  | 30  | 33  | 36  | 36    | UHT   |          |       |    |    |     |
| IF       | 2   | 2   | 2   | 5   | 5   | 5   | 7   | 9   | 13  | 20  | 23  | 23  | 25  | 29  | 31  | 33  | 34  | 32  | 31  | 30  | 29  | 22  | 19  | 16  | 20  | 27  | 30  | 33  | 33    | IF    |          |       |    |    |     |
| Position | 31  | 32  | 33  | 34  | 35  | 36  | 37  | 38  | 39  | 40  | 41  | 42  | 43  | 44  | 45  | 46  | 47  | 48  | 49  | 50  | 51  | 52  | 53  | 54  | 55  | 56  | 57  | 58  | 59    | 60    | Position |       |    |    |     |
| AA       | V   | F   | G   | K   | E   | K   | V   | N   | E   | L   | S   | K   | D   | I   | G   | S   | E   | S   | T   | E   | D   | Q   | A   | M   | E   | D   | I   | K   | Q     | M     | AA       |       |    |    |     |
| Total    | 36  | 36  | 34  | 30  | 27  | 23  | 20  | 15  | 15  | 13  | 12  | 8   | 10  | 11  | 11  | 11  | 11  | 11  | 11  | 11  | 11  | 11  | 10  | 10  | 10  | 10  | 10  | 10  | 0     | 0     | Total    |       |    |    |     |
| RM       | 36  | 36  | 34  | 30  | 27  | 23  | 20  | 15  | 15  | 13  | 12  | 8   | 10  | 11  | 11  | 11  | 11  | 11  | 11  | 11  | 11  | 11  | 10  | 10  | 10  | 10  | 10  | 10  | 10    | 10    | RM       |       |    |    |     |
| UHT      | 36  | 36  | 34  | 30  | 27  | 23  | 20  | 15  | 15  | 13  | 12  | 8   | 10  | 11  | 11  | 11  | 11  | 11  | 11  | 11  | 11  | 11  | 10  | 10  | 10  | 10  | 10  | 10  | 10    | 10    | UHT      |       |    |    |     |
| IF       | 33  | 33  | 31  | 29  | 26  | 23  | 20  | 15  | 15  | 13  | 12  | 8   | 9   | 9   | 9   | 9   | 9   | 9   | 9   | 9   | 9   | 8   | 8   | 8   | 8   | 8   | 8   | 8   | 8     | IF    |          |       |    |    |     |
| Position | 61  | 62  | 63  | 64  | 65  | 66  | 67  | 68  | 69  | 70  | 71  | 72  | 73  | 74  | 75  | 76  | 77  | 78  | 79  | 80  | 81  | 82  | 83  | 84  | 85  | 86  | 87  | 88  | 89    | 90    | Position |       |    |    |     |
| AA       | E   | A   | E   | S   | I   | S   | S   | S   | E   | E   | I   | V   | P   | N   | S   | V   | E   | Q   | K   | H   | I   | Q   | K   | E   | D   | V   | P   | S   | E     | R     | AA       |       |    |    |     |
| Total    | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 15  | 20  | 21  | 23  | 24  | 24  | 27  | 27  | 27  | 26    | Total |          |       |    |    |     |
| RM       |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     | 15  | 20  | 21  | 23  | 24  | 24  | 27  | 27  | 27  | 26    | RM    |          |       |    |    |     |
| UHT      |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     | 13  | 18  | 19  | 21  | 22  | 22  | 25  | 25  | 25  | 24    | UHT   |          |       |    |    |     |
| IF       |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     | 15  | 20  | 20  | 21  | 22  | 22  | 24  | 24  | 24  | 23    | IF    |          |       |    |    |     |
| Position | 91  | 92  | 93  | 94  | 95  | 96  | 97  | 98  | 99  | 100 | 101 | 102 | 103 | 104 | 105 | 106 | 107 | 108 | 109 | 110 | 111 | 112 | 113 | 114 | 115 | 116 | 117 | 118 | 119   | 120   | Position |       |    |    |     |
| AA       | Y   | L   | G   | Y   | L   | E   | Q   | L   | L   | R   | K   | K   | Y   | K   | V   | P   | Q   | L   | E   | I   | V   | N   | S   | A   | E   | E   | R   | L   | AA    |       |          |       |    |    |     |
| Total    | 28  | 26  | 28  | 27  | 28  | 27  | 26  | 24  | 22  | 18  | 14  | 10  | 12  | 18  | 25  | 37  | 37  | 42  | 45  | 47  | 48  | 49  | 49  | 50  | 50  | 50  | 50  | 50  | 50    | 36    | Total    |       |    |    |     |
| RM       | 28  | 26  | 28  | 27  | 28  | 27  | 26  | 24  | 22  | 18  | 14  | 10  | 12  | 17  | 22  | 34  | 34  | 39  | 42  | 44  | 45  | 46  | 46  | 47  | 47  | 47  | 47  | 47  | 33    | RM    |          |       |    |    |     |
| UHT      | 26  | 24  | 26  | 25  | 26  | 26  | 26  | 24  | 22  | 18  | 14  | 10  | 12  | 17  | 22  | 34  | 34  | 39  | 42  | 44  | 45  | 46  | 46  | 47  | 47  | 47  | 47  | 47  | 33    | UHT   |          |       |    |    |     |
| IF       | 23  | 20  | 20  | 20  | 21  | 20  | 19  | 17  | 16  | 14  | 10  | 8   | 11  | 18  | 25  | 37  | 37  | 42  | 44  | 46  | 47  | 48  | 48  | 48  | 48  | 48  | 48  | 34  | IF    |       |          |       |    |    |     |
| Position | 121 | 122 | 123 | 124 | 125 | 126 | 127 | 128 | 129 | 130 | 131 | 132 | 133 | 134 | 135 | 136 | 137 | 138 | 139 | 140 | 141 | 142 | 143 | 144 | 145 | 146 | 147 | 148 | 149   | 150   | Position |       |    |    |     |
| AA       | H   | S   | M   | K   | E   | G   | I   | H   | A   | Q   | Q   | K   | E   | P   | M   | I   | G   | V   | N   | Q   | E   | L   | A   | Y   | F   | Y   | P   | E   | L     | F     | AA       |       |    |    |     |
| Total    | 36  | 33  | 29  | 8   | 4   | 4   | 4   | 4   | 4   | 4   | 5   | 5   | 4   | 4   | 4   | 4   | 4   | 4   | 4   | 4   | 4   | 4   | 4   | 4   | 2   | 2   | 2   | 2   | 2     | 2     | 2        | Total |    |    |     |
| RM       | 33  | 31  | 27  | 8   | 4   | 4   | 4   | 4   | 4   | 4   | 4   | 3   | 2   | 2   | 2   | 2   | 2   | 2   | 2   | 2   | 2   | 2   | 2   | 2   | 2   | 2   | 2   | 2   | 2     | 2     | RM       |       |    |    |     |
| UHT      | 33  | 31  | 27  | 8   | 4   | 4   | 4   | 4   | 4   | 4   | 4   | 3   | 2   | 2   | 2   | 2   | 2   | 2   | 2   | 2   | 2   | 2   | 2   | 2   | 2   | 2   | 2   | 2   | 2     | 2     | UHT      |       |    |    |     |
| IF       | 34  | 31  | 27  | 8   | 3   | 3   | 3   | 3   | 3   | 4   | 4   | 3   | 3   | 3   | 3   | 3   | 3   | 3   | 3   | 3   | 3   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1     | IF    |          |       |    |    |     |
| Position | 151 | 152 | 153 | 154 | 155 | 156 | 157 | 158 | 159 | 160 | 161 | 162 | 163 | 164 | 165 | 166 | 167 | 168 | 169 | 170 | 171 | 172 | 173 | 174 | 175 | 176 | 177 | 178 | 179   | 180   | Position |       |    |    |     |
| AA       | R   | Q   | F   | Y   | Q   | L   | D   | A   | Y   | P   | S   | G   | A   | W   | Y   | V   | P   | L   | G   | T   | Q   | Y   | T   | D   | A   | P   | S   | F   | S     | AA    |          |       |    |    |     |
| Total    | 1   | 1   | 1   | 1   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 2   | 2   | 2   | 2   | 3   | 6   | 6   | 9   | 9   | 13  | 15  | 17  | 19  | 26  | Total |       |          |       |    |    |     |
| RM       | 1   | 1   | 1   | 1   |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     | 2   | 2   | 2   | 2   | 5   | 5   | 8   | 8   | 11  | 11    | 13    | 14       | 21    | RM |    |     |
| UHT      | 1   | 1   | 1   | 1   |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     | 2   | 2   | 2   | 2   | 3   | 6   | 6   | 9   | 9   | 9     | 13    | 15       | 17    | 19 | 26 | UHT |
| IF       | 1   | 1   | 1   | 1   |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     | 2   | 2   | 2   | 2   | 5   | 5   | 8   | 8   | 11  | 11    | 13    | 14       | 20    | IF |    |     |

**Figure S3:** Protein sequence of  $\alpha_{S1}$ -casein without the signal peptide. The numbers below the sequence indicate how many peptides containing this specific residue were detected over all samples (total) and in RM (sequence coverage 83.9 %), UHT milk (sequence coverage 83.9 %), and IF (sequence coverage 89.4 %). AA denotes amino acid.

| Position | 1   | 2   | 3   | 4   | 5   | 6   | 7   | 8   | 9   | 10  | 11  | 12  | 13  | 14  | 15  | 16  | 17  | 18  | 19  | 20  | 21  | 22  | 23  | 24  | 25  | 26  | 27  | 28       | 29            | 30    | Position |       |
|----------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|----------|---------------|-------|----------|-------|
| AA       | K   | N   | T   | M   | E   | H   | V   | S   | S   | I   | I   | S   | I   | I   | S   | Q   | E   | T   | Y   | K   | Q   | E   | K   | N   | M   | A   | I   | N        | P <th>AA</th> | AA    |          |       |
| Total    | 9   | 9   | 9   | 9   | 9   | 9   | 9   | 9   | 10  | 10  | 11  | 11  | 12  | 15  | 15  | 15  | 15  | 15  | 15  | 15  | 13  | 6   | 5   | 4   | 0   | 0   | 0   | 0        | 0             | Total |          |       |
| RM       | 9   | 9   | 9   | 9   | 9   | 9   | 9   | 9   | 9   | 10  | 10  | 10  | 10  | 10  | 13  | 13  | 13  | 13  | 13  | 13  | 13  | 11  | 6   | 5   | 4   | 0   | 0   | 0        | 0             | 0     | RM       |       |
| UHT      | 9   | 9   | 9   | 9   | 9   | 9   | 9   | 9   | 10  | 10  | 10  | 10  | 10  | 13  | 13  | 13  | 13  | 13  | 13  | 13  | 11  | 6   | 5   | 4   | 0   | 0   | 0   | 0        | 0             | UHT   |          |       |
| IF       | 9   | 9   | 9   | 9   | 9   | 9   | 9   | 9   | 10  | 10  | 11  | 11  | 12  | 15  | 15  | 15  | 15  | 15  | 15  | 15  | 13  | 6   | 5   | 4   | 0   | 0   | 0   | 0        | 0             | IF    |          |       |
| Position | 31  | 32  | 33  | 34  | 35  | 36  | 37  | 38  | 39  | 40  | 41  | 42  | 43  | 44  | 45  | 46  | 47  | 48  | 49  | 50  | 51  | 52  | 53  | 54  | 55  | 56  | 57  | 58       | 59            | 60    | Position |       |
| AA       | S   | K   | E   | N   | L   | C   | S   | T   | F   | C   | K   | E   | V   | V   | R   | A   | N   | E   | E   | E   | Y   | S   | I   | G   | S   | S   | S   | E        | E             | AA    |          |       |
| Total    | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0        | 0             | Total |          |       |
| RM       |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |          |               | RM    |          |       |
| UHT      |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |          |               | UHT   |          |       |
| IF       |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |          |               | IF    |          |       |
| Position | 61  | 62  | 63  | 64  | 65  | 66  | 67  | 68  | 69  | 70  | 71  | 72  | 73  | 74  | 75  | 76  | 77  | 78  | 79  | 80  | 81  | 82  | 83  | 84  | 85  | 86  | 87  | 88       | 89            | 90    | Position |       |
| AA       | S   | A   | E   | V   | A   | T   | E   | E   | V   | K   | I   | T   | V   | D   | D   | K   | H   | Y   | Q   | K   | A   | L   | N   | E   | I   | N   | Q   | F        | Y             | Q     | AA       |       |
| Total    | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 2   | 2   | 2   | 2   | 2   | 2   | 2   | 2   | 1   | 0   | 4   | 4   | 4   | 4   | 4   | 4   | 4   | 5        | 6             | 6     | Total    |       |
| RM       |     |     |     |     |     |     |     |     |     |     | 2   | 2   | 2   | 2   | 2   | 2   | 2   | 2   | 1   |     |     |     |     |     |     |     |     |          |               | RM    |          |       |
| UHT      |     |     |     |     |     |     |     |     |     |     | 2   | 2   | 2   | 2   | 2   | 2   | 2   | 2   | 1   |     |     |     |     |     |     |     |     |          |               | UHT   |          |       |
| IF       |     |     |     |     |     |     |     |     |     |     | 2   | 2   | 2   | 2   | 2   | 2   | 2   | 2   | 1   |     | 4   | 4   | 4   | 4   | 4   | 4   | 4   | 5        | 6             | 6     | IF       |       |
| Position | 91  | 92  | 93  | 94  | 95  | 96  | 97  | 98  | 99  | 100 | 101 | 102 | 103 | 104 | 105 | 106 | 107 | 108 | 109 | 110 | 111 | 112 | 113 | 114 | 115 | 116 | 117 | 118      | 119           | 120   | Position |       |
| AA       | K   | F   | P   | Q   | Y   | L   | Q   | Y   | L   | Y   | Q   | G   | P   | I   | V   | L   | N   | P   | W   | D   | Q   | K   | R   | N   | A   | V   | P   | I        | T             | AA    |          |       |
| Total    | 6   | 6   | 6   | 6   | 6   | 4   | 5   | 4   | 4   | 8   | 10  | 12  | 12  | 12  | 13  | 13  | 13  | 13  | 13  | 13  | 13  | 13  | 11  | 5   | 7   | 5   | 5   | 5        | 5             | 5     | 5        | Total |
| RM       |     |     |     |     |     |     | 1   | 3   | 5   | 7   | 9   | 9   | 9   | 10  | 10  | 10  | 10  | 10  | 10  | 10  | 10  | 10  | 9   | 3   | 4   | 4   | 4   | 4        | 4             | 4     | RM       |       |
| UHT      |     |     |     |     |     |     | 1   | 3   | 5   | 7   | 8   | 8   | 8   | 9   | 9   | 9   | 9   | 9   | 9   | 9   | 9   | 9   | 9   | 3   | 5   | 5   | 5   | 5        | 5             | 5     | UHT      |       |
| IF       |     |     |     |     |     |     | 6   | 6   | 4   | 4   | 3   | 7   | 9   | 10  | 10  | 11  | 11  | 11  | 11  | 11  | 11  | 11  | 10  | 5   | 7   | 5   | 5   | 5        | 5             | 5     | IF       |       |
| Position | 121 | 122 | 123 | 124 | 125 | 126 | 127 | 128 | 129 | 130 | 131 | 132 | 133 | 134 | 135 | 136 | 137 | 138 | 139 | 140 | 141 | 142 | 143 | 144 | 145 | 146 | 147 | 148      | 149           | 150   | Position |       |
| AA       | P   | T   | L   | N   | R   | E   | Q   | L   | S   | T   | S   | E   | N   | S   | K   | K   | T   | V   | D   | M   | E   | S   | T   | E   | V   | F   | T   | K        | K             | AA    |          |       |
| Total    | 5   | 5   | 9   | 9   | 9   | 9   | 9   | 9   | 8   | 8   | 8   | 8   | 8   | 8   | 9   | 6   | 9   | 12  | 16  | 18  | 21  | 21  | 21  | 21  | 21  | 21  | 21  | 21       | 8             | Total |          |       |
| RM       | 4   | 4   | 8   | 8   | 8   | 8   | 8   | 8   | 8   | 8   | 8   | 8   | 8   | 8   | 9   | 6   | 9   | 12  | 16  | 18  | 20  | 20  | 20  | 20  | 20  | 20  | 20  | 8        | RM            |       |          |       |
| UHT      | 5   | 5   | 9   | 9   | 9   | 9   | 9   | 9   | 8   | 8   | 8   | 8   | 8   | 8   | 9   | 6   | 9   | 12  | 16  | 18  | 20  | 20  | 20  | 20  | 20  | 20  | 20  | UHT      |               |       |          |       |
| IF       | 5   | 5   | 9   | 9   | 9   | 9   | 9   | 9   | 8   | 8   | 8   | 8   | 8   | 8   | 9   | 6   | 9   | 11  | 13  | 14  | 17  | 17  | 17  | 17  | 17  | 17  | 17  | 5        | IF            |       |          |       |
| Position | 151 | 152 | 153 | 154 | 155 | 156 | 157 | 158 | 159 | 160 | 161 | 162 | 163 | 164 | 165 | 166 | 167 | 168 | 169 | 170 | 171 | 172 | 173 | 174 | 175 | 176 | 177 | 178      | 179           | 180   | Position |       |
| AA       | T   | K   | L   | T   | E   | E   | E   | K   | N   | R   | L   | F   | L   | K   | K   | I   | S   | Q   | R   | Y   | Q   | K   | F   | A   | L   | P   | Q   | Y        | L             | AA    |          |       |
| Total    | 7   | 10  | 13  | 16  | 17  | 17  | 17  | 17  | 17  | 17  | 17  | 15  | 11  | 6   | 1   | 1   | 1   | 1   | 3   | 5   | 5   | 7   | 8   | 10  | 10  | 10  | 10  | 7        | 7             | Total |          |       |
| RM       | 7   | 10  | 13  | 16  | 17  | 17  | 17  | 17  | 17  | 17  | 17  | 15  | 14  | 10  | 5   |     |     |     | 1   | 2   | 2   | 4   | 5   | 7   | 7   | 7   | 7   | 7        | RM            |       |          |       |
| UHT      | 7   | 10  | 13  | 16  | 17  | 17  | 17  | 17  | 17  | 17  | 17  | 15  | 14  | 10  | 5   |     |     |     | 1   | 2   | 2   | 4   | 5   | 7   | 7   | 7   | 7   | 7        | UHT           |       |          |       |
| IF       | 7   | 9   | 12  | 15  | 16  | 16  | 16  | 16  | 16  | 16  | 15  | 14  | 10  | 5   | 1   | 1   | 1   | 1   | 3   | 5   | 5   | 6   | 6   | 7   | 7   | 7   | 7   | 4        | IF            |       |          |       |
| Position | 181 | 182 | 183 | 184 | 185 | 186 | 187 | 188 | 189 | 190 | 191 | 192 | 193 | 194 | 195 | 196 | 197 | 198 | 199 | 200 | 201 | 202 | 203 | 204 | 205 | 206 | 207 | Position |               |       |          |       |
| AA       | K   | T   | V   | Y   | Q   | H   | Q   | K   | A   | M   | K   | P   | W   | I   | Q   | P   | K   | T   | K   | V   | I   | P   | Y   | V   | R   | Y   | L   | AA       |               |       |          |       |
| Total    | 5   | 4   | 4   | 3   | 3   | 2   | 2   | 1   | 6   | 6   | 7   | 7   | 7   | 7   | 7   | 5   | 8   | 8   | 10  | 11  | 11  | 10  | 10  | 10  | 9   | 7   | 4   | Total    |               |       |          |       |
| RM       | 5   | 4   | 4   | 3   | 3   | 2   | 2   | 1   | 4   | 4   | 5   | 5   | 5   | 5   | 5   | 3   | 7   | 9   | 10  | 10  | 10  | 10  | 10  | 9   | 7   | 4   | RM  |          |               |       |          |       |
| UHT      | 5   | 4   | 4   | 3   | 3   | 2   | 2   | 1   | 4   | 4   | 5   | 5   | 5   | 5   | 5   | 3   | 7   | 7   | 9   | 10  | 10  | 10  | 10  | 9   | 7   | 4   | UHT |          |               |       |          |       |
| IF       | 2   | 1   | 1   | 1   | 1   |     |     |     | 4   | 4   | 4   | 4   | 4   | 4   | 4   | 3   | 6   | 6   | 8   | 9   | 9   | 8   | 7   | 6   | 4   |     | IF  |          |               |       |          |       |

**Figure S4:** Protein sequence of  $\alpha_{S2}$ -casein without the signal peptide. The numbers below the sequence indicate how many peptides containing this specific residue were detected over all samples (total) and in RM (sequence coverage 66.7 %), UHT milk (sequence coverage 66.7 %), and IF (sequence coverage 75.8 %). AA denotes amino acid.

| Position | 1   | 2   | 3   | 4   | 5   | 6   | 7   | 8   | 9   | 10  | 11  | 12  | 13  | 14  | 15  | 16  | 17  | 18  | 19  | 20  | 21  | 22  | 23  | 24  | 25  | 26  | 27  | 28  | 29  | 30    | Position |
|----------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-------|----------|
| AA       | I   | L   | N   | K   | P   | E   | D   | E   | T   | H   | L   | E   | A   | Q   | P   | T   | D   | A   | S   | A   | Q   | F   | I   | R   | N   | L   | Q   | I   | S   | N     | AA       |
| Total    | 15  | 18  | 18  | 18  | 18  | 18  | 18  | 18  | 18  | 18  | 18  | 18  | 18  | 18  | 18  | 17  | 16  | 15  | 15  | 14  | 13  | 9   | 8   | 5   | 4   | 2   | 1   | 1   | 1   | Total |          |
| RM       | 14  | 17  | 17  | 17  | 17  | 17  | 17  | 17  | 17  | 17  | 17  | 15  | 15  | 15  | 15  | 14  | 13  | 12  | 12  | 11  | 10  | 8   | 7   | 4   | 3   | 2   | 1   | 1   | 1   | RM    |          |
| UHT      | 15  | 18  | 18  | 18  | 18  | 18  | 18  | 18  | 18  | 18  | 18  | 17  | 15  | 15  | 15  | 15  | 14  | 13  | 12  | 12  | 11  | 10  | 8   | 7   | 4   | 3   | 2   | 1   | 1   | 1     | UHT      |
| IF       | 15  | 17  | 17  | 17  | 17  | 17  | 17  | 17  | 17  | 17  | 17  | 17  | 17  | 17  | 17  | 16  | 15  | 14  | 14  | 13  | 12  | 8   | 7   | 5   | 4   | 2   | 1   | 1   | 1   | IF    |          |
| Position | 31  | 32  | 33  | 34  | 35  | 36  | 37  | 38  | 39  | 40  | 41  | 42  | 43  | 44  | 45  | 46  | 47  | 48  | 49  | 50  | 51  | 52  | 53  | 54  | 55  | 56  | 57  | 58  | 59  | 60    | Position |
| AA       | E   | D   | L   | S   | K   | E   | P   | S   | I   | S   | R   | E   | D   | L   | I   | S   | K   | E   | Q   | I   | V   | I   | R   | S   | S   | R   | Q   | P   | Q   | S     | AA       |
| Total    | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 2   | 2   | 2   | 2   | 2   | 2   | 2   | 2   | 2   | 2   | 8   | 11  | 11  | 16  | 16  | 16  | 19    | Total    |
| RM       | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 2   | 2   | 2   | 2   | 2   | 2   | 2   | 2   | 2   | 8   | 11  | 11  | 16  | 16  | 16  | 16    | RM       |
| UHT      | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 2   | 2   | 2   | 2   | 2   | 2   | 2   | 2   | 2   | 8   | 11  | 11  | 16  | 16  | 16  | 17    | UHT      |
| IF       | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 2   | 2   | 2   | 2   | 2   | 2   | 2   | 2   | 2   | 2   | 8   | 11  | 11  | 14  | 14  | 14  | 17    | IF       |
| Position | 61  | 62  | 63  | 64  | 65  | 66  | 67  | 68  | 69  | 70  | 71  | 72  | 73  | 74  | 75  | 76  | 77  | 78  | 79  | 80  | 81  | 82  | 83  | 84  | 85  | 86  | 87  | 88  | 89  | 90    | Position |
| AA       | Q   | N   | P   | K   | L   | P   | L   | S   | I   | L   | K   | E   | K   | H   | L   | R   | N   | A   | T   | L   | G   | S   | E   | E   | T   | T   | E   | H   | T   | P     | AA       |
| Total    | 19  | 20  | 21  | 21  | 24  | 24  | 23  | 21  | 17  | 17  | 11  | 8   | 7   | 4   | 3   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | Total |          |
| RM       | 16  | 16  | 16  | 16  | 19  | 19  | 18  | 17  | 14  | 14  | 11  | 8   | 7   | 4   | 3   |     |     |     |     |     |     |     |     |     |     |     |     |     |     |       | RM       |
| UHT      | 17  | 17  | 17  | 17  | 20  | 20  | 19  | 17  | 14  | 14  | 11  | 8   | 7   | 4   | 3   |     |     |     |     |     |     |     |     |     |     |     |     |     |     |       | UHT      |
| IF       | 17  | 18  | 19  | 19  | 20  | 20  | 19  | 17  | 13  | 13  | 7   | 5   | 4   | 2   | 2   |     |     |     |     |     |     |     |     |     |     |     |     |     |     |       | IF       |
| Position | 91  | 92  | 93  | 94  | 95  | 96  | 97  | 98  | 99  | 100 | 101 | 102 | 103 | 104 | 105 | 106 | 107 | 108 | 109 | 110 | 111 | 112 | 113 | 114 | 115 | 116 | 117 | 118 | 119 | 120   | Position |
| AA       | S   | D   | A   | S   | T   | T   | E   | G   | K   | L   | M   | E   | L   | G   | H   | K   | I   | M   | R   | N   | L   | E   | N   | T   | V   | K   | E   | T   | I   | K     | AA       |
| Total    | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 1   | 1   | 2   | 3   | 4   | 4   | 4   | 4   | 4   | 4   | 4   | Total |          |
| RM       |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     | RM    |          |
| UHT      |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     | UHT   |          |
| IF       |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     | IF    |          |
| Position | 121 | 122 | 123 | 124 | 125 | 126 | 127 | 128 | 129 | 130 | 131 | 132 | 133 | 134 | 135 |     |     |     |     |     |     |     |     |     |     |     |     |     |     |       | Position |
| AA       | Y   | L   | K   | S   | L   | F   | S   | H   | A   | F   | E   | V   | V   | K   | T   |     |     |     |     |     |     |     |     |     |     |     |     |     |     | AA    |          |
| Total    | 4   | 1   | 2   | 3   | 3   | 4   | 5   | 6   | 6   | 6   | 6   | 6   | 6   | 6   | 6   |     |     |     |     |     |     |     |     |     |     |     |     |     |     | Total |          |
| RM       |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     | RM    |          |
| UHT      |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     | UHT   |          |
| IF       |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     | IF    |          |

**Figure S5:** Protein sequence of GlyCAM-1 without the signal peptide. The numbers below the sequence indicate how many peptides containing this specific residue were detected over all samples (total) and in RM (sequence coverage 62.2 %), UHT milk (sequence coverage 74.1 %), and IF (sequence coverage 75.6 %). AA denotes amino acid.

| Position | 1   | 2   | 3   | 4   | 5   | 6   | 7   | 8   | 9   | 10  | 11  | 12  | 13  | 14  | 15  | 16  | 17  | 18  | 19  | 20  | 21  | 22  | 23  | 24  | 25  | 26  | 27  | 28  | 29  | 30       | Position |
|----------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|----------|----------|
| AA       | Q   | E   | Q   | N   | Q   | E   | Q   | P   | I   | R   | C   | E   | K   | D   | E   | R   | F   | F   | S   | D   | K   | I   | A   | K   | Y   | I   | P   | I   | Q   | Y        | AA       |
| Total    | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 0   | 0   | 0   | 0   | 0        | Total    |
| RM       |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1        | RM       |
| UHT      |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1        | UHT      |
| IF       |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1        | IF       |
| Position | 31  | 32  | 33  | 34  | 35  | 36  | 37  | 38  | 39  | 40  | 41  | 42  | 43  | 44  | 45  | 46  | 47  | 48  | 49  | 50  | 51  | 52  | 53  | 54  | 55  | 56  | 57  | 58  | 59  | 60       | Position |
| AA       | V   | L   | S   | R   | Y   | P   | S   | Y   | G   | L   | N   | Y   | Y   | Q   | Q   | K   | P   | V   | A   | L   | I   | N   | N   | Q   | F   | L   | P   | Y   | P   | Y        | AA       |
| Total    | 4   | 4   | 7   | 7   | 7   | 7   | 7   | 7   | 6   | 6   | 5   | 5   | 7   | 5   | 5   | 5   | 5   | 5   | 6   | 6   | 4   | 5   | 5   | 3   | 3   | 3   | 3   | 3   | 3   | Total    |          |
| RM       |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | RM       |          |
| UHT      |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | UHT |          |          |
| IF       | 4   | 4   | 7   | 7   | 7   | 7   | 7   | 7   | 6   | 6   | 5   | 5   | 7   | 5   | 5   | 5   | 5   | 5   | 5   | 3   | 4   | 4   | 2   | 2   | 2   | 2   | 2   | 2   | IF  |          |          |
| Position | 61  | 62  | 63  | 64  | 65  | 66  | 67  | 68  | 69  | 70  | 71  | 72  | 73  | 74  | 75  | 76  | 77  | 78  | 79  | 80  | 81  | 82  | 83  | 84  | 85  | 86  | 87  | 88  | 89  | 90       | Position |
| AA       | Y   | A   | K   | P   | A   | A   | V   | R   | S   | P   | A   | Q   | I   | L   | Q   | W   | Q   | V   | L   | S   | N   | T   | V   | P   | A   | K   | S   | C   | Q   | A        | AA       |
| Total    | 3   | 3   | 3   | 3   | 3   | 2   | 2   | 2   | 3   | 3   | 3   | 3   | 3   | 3   | 2   | 2   | 1   | 1   | 1   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | Total    |          |
| RM       | 1   | 1   | 1   | 1   | 1   |     |     |     | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   |     |     |     |     |     |     |     |     |     | RM  |          |          |
| UHT      | 1   | 1   | 1   | 1   | 1   |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     | UHT |          |          |
| IF       | 2   | 2   | 2   | 2   | 2   | 2   | 2   | 2   | 2   | 2   | 2   | 2   | 2   | 2   | 2   | 2   | 2   | 1   | 1   |     |     |     |     |     |     |     |     |     | IF  |          |          |
| Position | 91  | 92  | 93  | 94  | 95  | 96  | 97  | 98  | 99  | 100 | 101 | 102 | 103 | 104 | 105 | 106 | 107 | 108 | 109 | 110 | 111 | 112 | 113 | 114 | 115 | 116 | 117 | 118 | 119 | 120      | Position |
| AA       | Q   | P   | T   | T   | M   | A   | R   | H   | P   | H   | P   | H   | L   | S   | F   | M   | A   | I   | P   | P   | K   | K   | N   | Q   | D   | K   | T   | E   | I   | P        | AA       |
| Total    | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 3   | 3   | 3   | 3   | 3   | 3   | 3   | 3   | 4   | 4   | 4   | 4   | 4   | 4        | Total    |
| RM       |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     | RM  |          |          |
| UHT      |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     | UHT |          |          |
| IF       | 3   | 3   | 3   | 3   | 3   | 3   | 3   | 3   | 3   | 3   | 3   | 3   | 3   | 3   | 3   | 3   | 3   | 3   | 3   | 3   | 3   | 3   | 3   | 3   | 4   | 4   | 4   | 4   | 4   | IF       |          |
| Position | 121 | 122 | 123 | 124 | 125 | 126 | 127 | 128 | 129 | 130 | 131 | 132 | 133 | 134 | 135 | 136 | 137 | 138 | 139 | 140 | 141 | 142 | 143 | 144 | 145 | 146 | 147 | 148 | 149 | 150      | Position |
| AA       | T   | I   | N   | T   | I   | A   | S   | G   | E   | P   | T   | S   | T   | P   | T   | T   | E   | A   | V   | E   | S   | T   | V   | A   | T   | L   | E   | D   | S   | P        | AA       |
| Total    | 4   | 4   | 4   | 3   | 3   | 3   | 3   | 3   | 3   | 3   | 3   | 3   | 3   | 3   | 3   | 3   | 3   | 3   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 2   | 4   | 5   | Total    |          |
| RM       |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     | 2   | 3   | RM       |          |
| UHT      |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     | 1   | 3   | 4        | UHT      |
| IF       | 4   | 4   | 4   | 3   | 3   | 3   | 3   | 3   | 3   | 3   | 3   | 3   | 3   | 3   | 3   | 3   | 3   | 3   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 2   | 4   | 5   | IF       |          |
| Position | 151 | 152 | 153 | 154 | 155 | 156 | 157 | 158 | 159 | 160 | 161 | 162 | 163 | 164 | 165 | 166 | 167 | 168 | 169 |     |     |     |     |     |     |     |     |     |     | Position |          |
| AA       | E   | V   | I   | E   | S   | P   | P   | E   | I   | N   | T   | V   | Q   | V   | T   | S   | T   | A   | V   |     |     |     |     |     |     |     |     |     |     | AA       |          |
| Total    | 6   | 9   | 9   | 9   | 10  | 10  | 10  | 10  | 11  | 11  | 11  | 10  | 10  | 10  | 10  | 10  | 10  | 10  | 10  | 10  |     |     |     |     |     |     |     |     |     | Total    |          |
| RM       | 3   | 4   | 4   | 4   | 4   | 4   | 4   | 4   | 4   | 4   | 4   | 3   | 3   | 3   | 3   | 3   | 3   | 3   | 3   |     |     |     |     |     |     |     |     | RM  |     |          |          |
| UHT      | 5   | 6   | 6   | 6   | 7   | 7   | 7   | 7   | 7   | 7   | 7   | 8   | 8   | 8   | 8   | 8   | 8   | 8   | 8   |     |     |     |     |     |     |     |     | UHT |     |          |          |
| IF       | 6   | 9   | 9   | 9   | 10  | 10  | 10  | 10  | 11  | 11  | 11  | 10  | 10  | 10  | 10  | 10  | 10  | 10  | 10  | 10  |     |     |     |     |     |     |     |     | IF  |          |          |

**Figure S6:** Protein sequence of κ-casein without the signal peptide. The numbers below the sequence indicate how many peptides containing this specific residue were detected over all samples (total) and in RM (sequence coverage 36.1 %), UHT milk (sequence coverage 29.6 %), and IF (sequence coverage 71.6 %). AA denotes amino acid.

| Position      | 1   | 2   | 3   | 4   | 5   | 6   | 7   | 8   | 9   | 10  | 11  | 12  | 13  | 14  | 15  | 16  | 17  | 18  | 19            | 20          | 21  | 22  | 23  | 24  | 25  | 26  | 27  | 28  | 29            | 30            | Position      | AA |    |    |    |  |
|---------------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|---------------|-------------|-----|-----|-----|-----|-----|-----|-----|-----|---------------|---------------|---------------|----|----|----|----|--|
| Total (unmod) | 2   | 2   | 2   | 6   | 6   | 6   | 8   | 10  | 14  | 21  | 25  | 25  | 27  | 31  | 33  | 36  | 37  | 35  | 34            | 33          | 31  | 24  | 22  | 18  | 22  | 30  | 33  | 36  | 36            | Total (unmod) |               |    |    |    |    |  |
| Total (mod)   | 10  | 10  | 10  | 10  | 10  | 10  | 10  | 10  | 10  | 10  | 10  | 10  | 10  | 10  | 9   | 9   | 9   | 8   | 8             | 8           | 7   | 6   | 6   | 11  | 17  | 20  | 20  | 21  | 21            | Total (mod)   |               |    |    |    |    |  |
| RM            | 4   | 4   | 4   | 4   | 4   | 4   | 4   | 4   | 4   | 4   | 4   | 4   | 4   | 4   | 4   | 4   | 4   | 4   | 4             | 4           | 3   | 1   |     |     |     |     |     |     | IF            |               |               |    |    |    |    |  |
| UHT           | 5   | 5   | 5   | 5   | 5   | 5   | 5   | 5   | 5   | 5   | 5   | 5   | 5   | 5   | 5   | 5   | 5   | 5   | 5             | 5           | 4   | 3   | 2   | 1   | 2   | 3   | 3   | 3   | 3             | 3             | IF            |    |    |    |    |  |
| IF            | 10  | 10  | 10  | 10  | 10  | 10  | 10  | 10  | 10  | 10  | 10  | 10  | 10  | 10  | 9   | 9   | 9   | 8   | 8             | 8           | 7   | 6   | 6   | 11  | 17  | 20  | 20  | 21  | 21            | IF            |               |    |    |    |    |  |
| Position      | 31  | 32  | 33  | 34  | 35  | 36  | 37  | 38  | 39  | 40  | 41  | 42  | 43  | 44  | 45  | 46  | 47  | 48  | 49            | 50          | 51  | 52  | 53  | 54  | 55  | 56  | 57  | 58  | 59            | 60            | Position      | AA |    |    |    |  |
| Total (unmod) | V   | F   | G   | K   | E   | K   | V   | N   | E   | L   | S   | K   | D   | I   | G   | S   | E   | S   | T             | E           | D   | Q   | A   | M   | E   | D   | I   | K   | Q             | M             | Total (unmod) |    |    |    |    |  |
| Total (mod)   | 36  | 36  | 34  | 30  | 27  | 23  | 20  | 15  | 15  | 13  | 12  | 8   | 10  | 11  | 11  | 11  | 11  | 11  | 11            | 11          | 11  | 11  | 11  | 10  | 10  | 10  | 10  | 0   | 0             | 0             | Total (mod)   |    |    |    |    |  |
| RM            | 3   | 3   | 3   | 3   | 3   | 3   | 3   | 3   | 3   | 3   | 3   | 3   | 0   | 0   | 0   | 0   | 0   | 0   | 0             | 0           | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0             | 0             | IF            |    |    |    |    |  |
| UHT           | 21  | 21  | 21  | 21  | 21  | 21  | 21  | 16  | 11  | 10  | 9   | 8   | 7   |     |     |     |     |     |               |             |     |     |     |     |     |     |     |     |               |               |               |    | IF |    |    |  |
| Position      | 61  | 62  | 63  | 64  | 65  | 66  | 67  | 68  | 69  | 70  | 71  | 72  | 73  | 74  | 75  | 76  | 77  | 78  | 79            | 80          | 81  | 82  | 83  | 84  | 85  | 86  | 87  | 88  | 89            | 90            | Position      | AA |    |    |    |  |
| Total (unmod) | E   | A   | S   | S   | S   | S   | E   | E   | E   | I   | V   | N   | S   | V   | E   | Q   | K   | H   | I             | O           | K   | E   | D   | V   | P   | S   | E   | R   | Total (unmod) |               |               |    |    |    |    |  |
| Total (mod)   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 15            | 20          | 21  | 23  | 24  | 24  | 27  | 27  | 27  | 27  | 26            | Total (mod)   |               |    |    |    |    |  |
| RM            |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     | 3             | 3           | 3   | 3   | 3   | 3   | 3   | 3   | 3   | 3   | 3             | 3             | 3             | 3  | 3  | 3  | IF |  |
| UHT           |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     | 9   | 11            | 11          | 11  | 11  | 11  | 11  | 11  | 11  | 11  | 11  | 11            | 11            | 11            | 11 | 11 | IF |    |  |
| IF            | 17  | 17  | 15  | 14  | 13  | 12  | 12  | 11  | 11  | 10  | 7   | 6   | 12  | 13  | 13  | 13  | 13  | 13  | 13            | 13          | 13  | 13  | 13  | 20  | 20  | 20  | 20  | 20  | 20            | 20            | IF            |    |    |    |    |  |
| Position      | 91  | 92  | 93  | 94  | 95  | 96  | 97  | 98  | 99  | 100 | 101 | 102 | 103 | 104 | 105 | 106 | 107 | 108 | 109           | 110         | 111 | 112 | 113 | 114 | 115 | 116 | 117 | 118 | 119           | 120           | Position      | AA |    |    |    |  |
| Total (unmod) | Y   | L   | G   | Y   | L   | E   | Q   | L   | R   | L   | K   | K   | Y   | K   | V   | P   | Q   | L   | E             | I           | V   | P   | N   | S   | A   | E   | E   | R   | Total (unmod) |               |               |    |    |    |    |  |
| Total (mod)   | 28  | 26  | 28  | 27  | 28  | 27  | 26  | 24  | 22  | 18  | 14  | 10  | 12  | 18  | 25  | 37  | 37  | 42  | 45            | 47          | 48  | 49  | 49  | 50  | 50  | 50  | 50  | 50  | 50            | 36            | Total (mod)   |    |    |    |    |  |
| RM            | 2   | 2   | 2   | 2   | 2   | 2   | 2   | 2   | 2   | 2   | 2   | 1   | 3   | 3   | 3   | 3   | 3   | 3   | 3             | 3           | 3   | 3   | 3   | 3   | 3   | 3   | 3   | 3   | 3             | 3             | IF            |    |    |    |    |  |
| UHT           | 9   | 7   | 7   | 6   | 6   | 6   | 6   | 6   | 6   | 6   | 4   | 3   | 9   | 9   | 8   | 8   | 8   | 8   | 8             | 8           | 8   | 8   | 8   | 8   | 8   | 8   | 8   | 8   | 8             | 8             | IF            |    |    |    |    |  |
| IF            | 17  | 15  | 14  | 13  | 12  | 12  | 11  | 11  | 10  | 7   | 6   | 12  | 13  | 13  | 13  | 13  | 13  | 13  | 13            | 13          | 13  | 13  | 13  | 13  | 13  | 13  | 13  | 13  | IF            |               |               |    |    |    |    |  |
| Position      | 121 | 122 | 123 | 124 | 125 | 126 | 127 | 128 | 129 | 130 | 131 | 132 | 133 | 134 | 135 | 136 | 137 | 138 | 139           | 140         | 141 | 142 | 143 | 144 | 145 | 146 | 147 | 148 | 149           | 150           | Position      | AA |    |    |    |  |
| Total (unmod) | H   | S   | M   | K   | E   | G   | I   | H   | A   | Q   | Q   | K   | E   | P   | M   | I   | G   | N   | Q             | E           | L   | A   | Y   | F   | P   | E   | L   | F   | Total (unmod) |               |               |    |    |    |    |  |
| Total (mod)   | 36  | 33  | 29  | 8   | 4   | 4   | 4   | 4   | 4   | 5   | 4   | 4   | 4   | 4   | 4   | 4   | 4   | 4   | 4             | 4           | 4   | 2   | 2   | 2   | 2   | 2   | 2   | 2   | 0             | Total (mod)   |               |    |    |    |    |  |
| RM            | 3   | 3   | 3   | 3   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0             | 0           | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0             | 0             | IF            |    |    |    |    |  |
| UHT           | 8   | 8   | 8   | 8   | 2   |     |     |     |     |     |     |     |     |     |     |     |     |     |               |             |     |     |     |     |     |     |     |     |               |               | IF            |    |    |    |    |  |
| IF            | 13  | 13  | 13  | 13  | 3   |     |     |     |     |     |     |     |     |     |     |     |     |     |               |             |     |     |     |     |     |     |     |     |               |               | IF            |    |    |    |    |  |
| Position      | 151 | 152 | 153 | 154 | 155 | 156 | 157 | 158 | 159 | 160 | 161 | 162 | 163 | 164 | 165 | 166 | 167 | 168 | 169           | 170         | 171 | 172 | 173 | 174 | 175 | 176 | 177 | 178 | 179           | 180           | Position      | AA |    |    |    |  |
| Total (unmod) | R   | Q   | F   | Y   | Q   | L   | D   | A   | Y   | P   | S   | G   | A   | W   | Y   | V   | P   | L   | G             | T           | Q   | Y   | T   | D   | A   | P   | S   | F   | S             | Total (unmod) |               |    |    |    |    |  |
| Total (mod)   | 1   | 1   | 1   | 1   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 2   | 2   | 2   | 2   | 3             | 6           | 6   | 9   | 9   | 13  | 15  | 17  | 19  | 26  | Total (mod)   |               |               |    |    |    |    |  |
| RM            |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |               |             |     |     |     |     |     |     |     |     |               |               |               | IF |    |    |    |  |
| UHT           |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |               |             |     |     |     |     |     |     |     |     |               |               |               |    | IF |    |    |  |
| IF            | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0             | 0           | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0             | 0             | IF            |    |    |    |    |  |
| Position      | 181 | 182 | 183 | 184 | 185 | 186 | 187 | 188 | 189 | 190 | 191 | 192 | 193 | 194 | 195 | 196 | 197 | 198 | 199           | Position    | AA  |     |     |     |     |     |     |     |               |               |               |    |    |    |    |  |
| Total (unmod) | D   | I   | P   | N   | P   | I   | G   | S   | E   | N   | S   | E   | T   | T   | M   | P   | L   | W   | Total (unmod) |             |     |     |     |     |     |     |     |     |               |               |               |    |    |    |    |  |
| Total (mod)   | 30  | 36  | 38  | 42  | 48  | 51  | 51  | 53  | 55  | 57  | 58  | 59  | 60  | 57  | 55  | 55  | 43  | 41  | 41            | Total (mod) |     |     |     |     |     |     |     |     |               |               |               |    |    |    |    |  |
| RM            |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |               |             |     |     |     |     |     |     |     |     |               |               |               | IF |    |    |    |  |
| UHT           |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |               |             |     |     |     |     |     |     |     |     |               |               |               |    | IF |    |    |  |
| IF            | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0             | 0           | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0             | 0             | IF            |    |    |    |    |  |

**Figure S7:** Protein sequence of  $\alpha_{S1}$ -casein without the signal peptide. The numbers below the sequence indicate how many peptides containing this specific residue were detected in all samples as unmodified (unmod) and/or modified (mod) in RM, UHT milk, and IF. Lysine residues of the protein are framed with a dotted line, and modification sites are fully framed.

| Position      | 1   | 2   | 3   | 4   | 5   | 6   | 7   | 8   | 9   | 10  | 11  | 12  | 13  | 14  | 15  | 16  | 17  | 18  | 19  | 20  | 21  | 22  | 23  | 24  | 25  | 26  | 27  | 28  | 29  | 30            | Position      |     |
|---------------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|---------------|---------------|-----|
| AA            | I   | L   | N   | K   | P   | E   | D   | E   | T   | H   | L   | E   | A   | Q   | P   | T   | D   | A   | S   | A   | Q   | F   | I   | R   | N   | L   | Q   | I   | S   | N <th>AA</th> | AA            |     |
| Total (unmod) | 15  | 18  | 18  | 18  | 18  | 18  | 18  | 18  | 18  | 18  | 18  | 18  | 18  | 18  | 18  | 18  | 17  | 16  | 15  | 15  | 14  | 13  | 9   | 8   | 5   | 4   | 2   | 1   | 1   | 1             | Total (unmod) |     |
| Total (mod)   | 6   | 7   | 7   | 7   | 7   | 7   | 7   | 7   | 7   | 7   | 6   | 5   | 4   | 3   | 3   | 3   | 2   | 2   | 2   | 2   | 2   | 1   | 1   | 0   | 0   | 0   | 0   | 0   | 0   | Total (mod)   |               |     |
| RM            | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | RM            |               |     |
| UHT           | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | UHT           |               |     |
| IF            | 6   | 7   | 7   | 7   | 7   | 7   | 7   | 7   | 7   | 7   | 6   | 5   | 4   | 3   | 3   | 3   | 2   | 2   | 2   | 2   | 2   | 1   | 1   |     |     |     |     |     |     | IF            |               |     |
| Position      | 31  | 32  | 33  | 34  | 35  | 36  | 37  | 38  | 39  | 40  | 41  | 42  | 43  | 44  | 45  | 46  | 47  | 48  | 49  | 50  | 51  | 52  | 53  | 54  | 55  | 56  | 57  | 58  | 59  | 60            | Position      |     |
| AA            | E   | D   | L   | S   | K   | E   | P   | S   | I   | S   | R   | E   | D   | L   | I   | S   | K   | E   | Q   | I   | V   | I   | R   | S   | S   | R   | Q   | P   | Q   | S             | AA            |     |
| Total (unmod) | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 1   | 2   | 2   | 2   | 2   | 2   | 2   | 2   | 2   | 2   | 2   | 8   | 11  | 11  | 16  | 16  | 16  | 19            | Total (unmod) |     |
| Total (mod)   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 9   | 9   | 9   | 9   | 9   | 9   | 9             | Total (mod)   |     |
| RM            |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     | 2   | 2   | 2   | 2   | 2   | 2             | 2             | RM  |
| UHT           |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     | 9   | 9   | 9   | 9   | 9   | 9             | 9             | UHT |
| IF            |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |               | IF            |     |
| Position      | 61  | 62  | 63  | 64  | 65  | 66  | 67  | 68  | 69  | 70  | 71  | 72  | 73  | 74  | 75  | 76  | 77  | 78  | 79  | 80  | 81  | 82  | 83  | 84  | 85  | 86  | 87  | 88  | 89  | 90            | Position      |     |
| AA            | Q   | N   | P   | K   | L   | P   | L   | S   | I   | L   | K   | E   | K   | H   | L   | R   | N   | A   | T   | L   | G   | S   | E   | E   | T   | T   | E   | H   | T   | P             | AA            |     |
| Total (unmod) | 19  | 20  | 21  | 21  | 24  | 24  | 23  | 21  | 17  | 17  | 11  | 8   | 7   | 4   | 3   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | Total (unmod) |               |     |
| Total (mod)   | 9   | 9   | 9   | 9   | 9   | 9   | 9   | 8   | 8   | 8   | 7   | 6   | 6   | 2   | 2   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | Total (mod)   |               |     |
| RM            | 2   | 2   | 2   | 2   | 2   | 2   | 2   | 2   | 2   | 2   | 2   | 2   | 2   | 2   | 2   |     |     |     |     |     |     |     |     |     |     |     |     |     |     |               | RM            |     |
| UHT           |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |               | UHT           |     |
| IF            | 9   | 9   | 9   | 9   | 9   | 9   | 9   | 8   | 8   | 8   | 7   | 6   | 6   | 2   | 2   |     |     |     |     |     |     |     |     |     |     |     |     |     |     |               | IF            |     |
| Position      | 91  | 92  | 93  | 94  | 95  | 96  | 97  | 98  | 99  | 100 | 101 | 102 | 103 | 104 | 105 | 106 | 107 | 108 | 109 | 110 | 111 | 112 | 113 | 114 | 115 | 116 | 117 | 118 | 119 | 120           | Position      |     |
| AA            | S   | D   | A   | S   | T   | T   | E   | G   | K   | L   | M   | E   | L   | G   | H   | K   | I   | M   | R   | N   | L   | E   | N   | T   | V   | K   | E   | T   | I   | K             | AA            |     |
| Total (unmod) | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 1   | 1   | 2   | 3   | 4   | 4   | 4   | 4   | 4   | 4   | 4   | 4   | Total (unmod) |               |     |
| Total (mod)   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 0   | 2   | 2   | 4   | 6   | 6   | 6   | 6   | 6   | 6   | 6   | 6   | 6   | 6   | Total (mod)   |               |     |
| RM            |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |               | RM            |     |
| UHT           |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |               | UHT           |     |
| IF            | 6   |     | 1   | 1   | 1   | 3   | 4   | 4   | 4   | 4   | 4   | 4   | 4   | 4   | 4   | 4   |     |     |     |     |     |     |     |     |     |     |     |     |     |               | IF            |     |
| Position      | 121 | 122 | 123 | 124 | 125 | 126 | 127 | 128 | 129 | 130 | 131 | 132 | 133 | 134 | 135 |     |     |     |     |     |     |     |     |     |     |     |     |     |     | Position      |               |     |
| AA            | Y   | L   | K   | S   | L   | F   | S   | H   | A   | F   | E   | V   | V   | K   | T   |     |     |     |     |     |     |     |     |     |     |     |     |     |     | AA            |               |     |
| Total (unmod) | 4   | 1   | 2   | 3   | 3   | 4   | 5   | 6   | 6   | 6   | 6   | 6   | 6   | 6   | 6   |     |     |     |     |     |     |     |     |     |     |     |     |     |     | Total (unmod) |               |     |
| Total (mod)   | 6   | 0   | 1   | 1   | 1   | 3   | 4   | 4   | 4   | 4   | 4   | 4   | 4   | 4   | 4   |     |     |     |     |     |     |     |     |     |     |     |     |     |     | Total (mod)   |               |     |
| RM            |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |               | RM            |     |
| UHT           |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |               | UHT           |     |
| IF            | 6   |     | 1   | 1   | 1   | 3   | 4   | 4   | 4   | 4   | 4   | 4   | 4   | 4   | 4   |     |     |     |     |     |     |     |     |     |     |     |     |     |     | IF            |               |     |

**Figure S8:** Protein sequence of GlyCAM-1 without the signal peptide. The numbers below the sequence indicate how many peptides containing this specific residue were detected in all samples as unmodified (unmod) and/or modified (mod) in RM, UHT milk, and IF. Lysine residues of the protein are framed with a dotted line, and modification sites are fully framed.