

## Supplemental Information

### Top-down characterization of histone H4 proteoforms with ProteinGoggle 2.0

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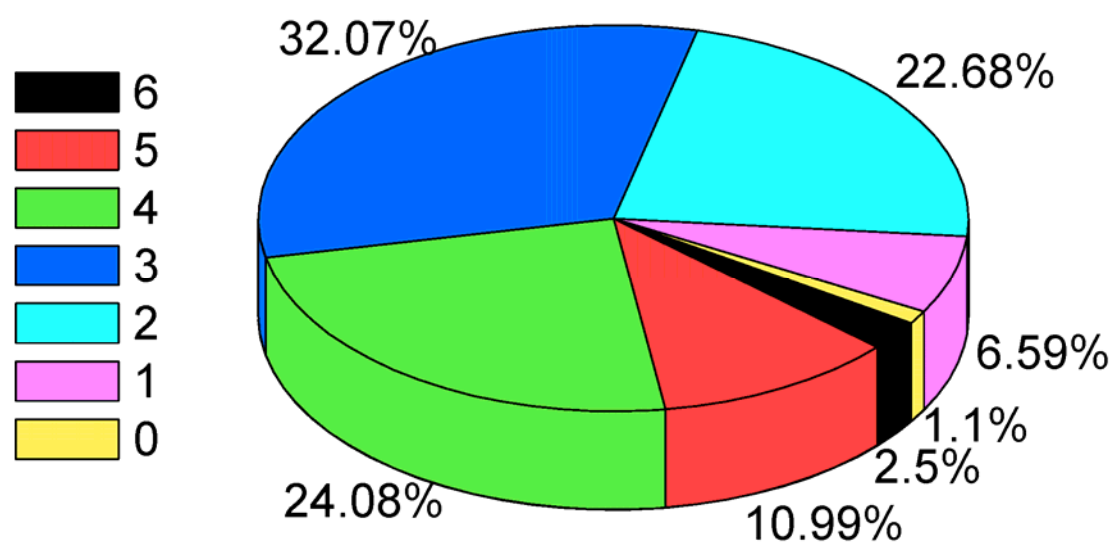
#### Contents

**Figure S1.** Distribution of number of PTMs per proteoform for the 365 proteoforms identified by ProteinGoggle 2.0.

**Figure S2.** Plot of number of acetylation per proteoform vs. elution time

**Figure S3.** The iEF map (A) and graphical fragmentation map (B) for the proteoform with S1AcK12AcY88P.

**Table S1.** The detailed information (including Spectrum Index, Retention Time (min), Isolation  $m/z$ , Experimental  $m/z$ , Theoretical  $m/z$ , IPMD (ppm),  $z$ , Theoretical monoisotopic mass (Da), Sequence, PTMs, Number of MPs, Number of non-MPs, P Score, PTM Score, Proteoform Score for each of the 426 H4 proteoforms.



**Figure S1.** Distribution of number of PTMs per proteoform for the 365 proteoforms identified by ProteinGoggle 2.0.

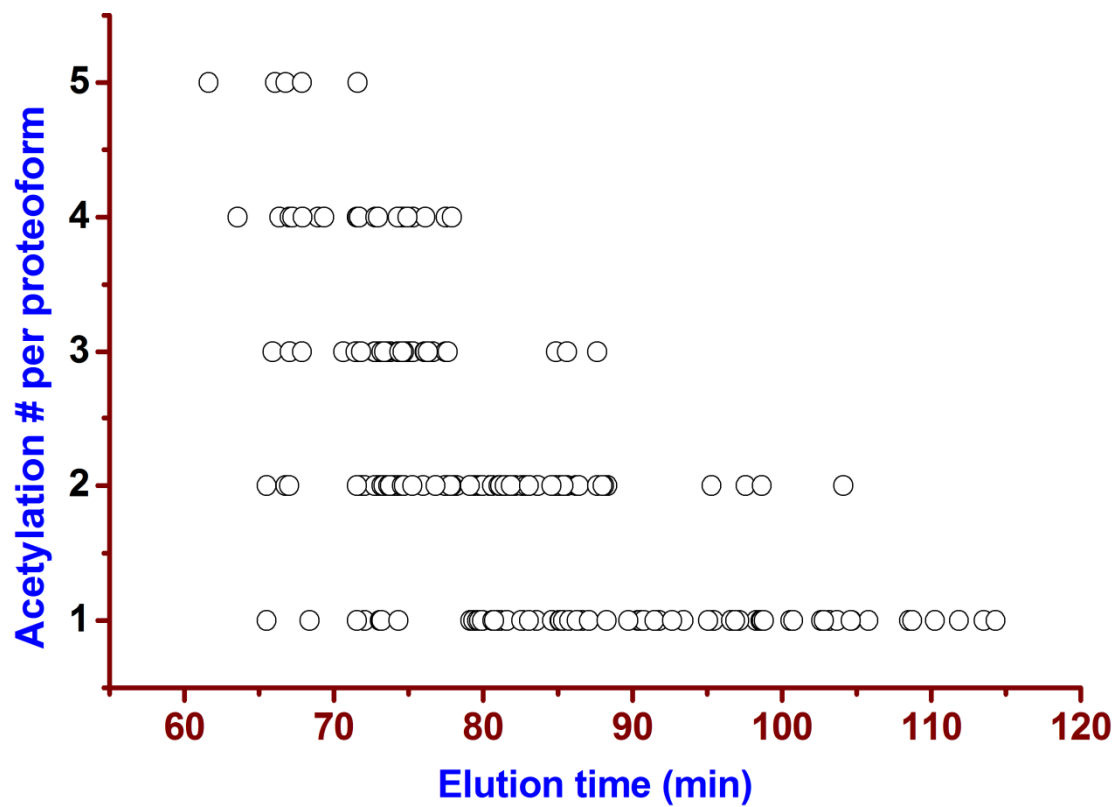
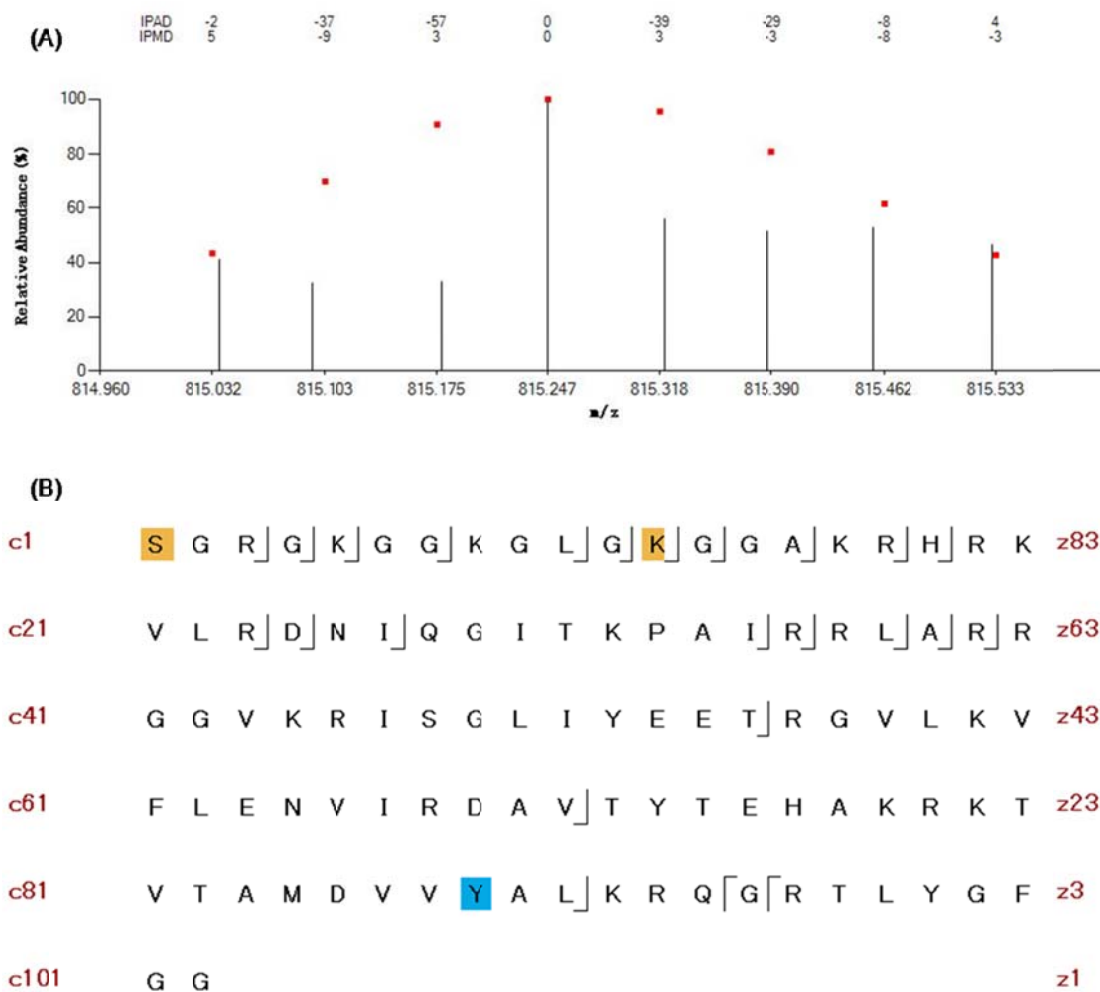


Figure S2. Plot of number of acetylation per proteoform vs. elution time.



**Figure S3.** The iEF map (A) and graphical fragmentation map (B) for the proteoform with S1AcK12AcY88P.

**Table S1.** The detailed information (including Spectrum Index, Retention Time (min), Isolation  $m/z$ , Experimental  $m/z$ , Theoretical  $m/z$ , IPMD (ppm),  $z$ , Theoretical monoisotopic mass (Da), Sequence, PTMs, Number of MPs, Number of non-MPs, P Score, PTM Score, Proteoform Score for each of the 426 H4 proteoforms.

| Spectrum Index | RT (min) | Iso. $m/z$ | Exp. $m/z$ | Theo. $m/z$ | IPMD (ppm) | $z$ | Theo. MM (Da) | Sequence | PTMs                          | MPs | non-MPs | P Score | PTM Score                 | Proteoform Score |
|----------------|----------|------------|------------|-------------|------------|-----|---------------|----------|-------------------------------|-----|---------|---------|---------------------------|------------------|
| 1326           | 61.62    | 882.5      | 884.6529   | 884.6583    | -6.14919   | 13  | 11483.55      | normal   | S1AcK5AcK8AcK12AcK16AcK20tMe  | 19  | 9       | 267.81  | S,0;K,0;K,0;K,0;K,4;      | 17               |
| 1326           | 61.62    | 882.5      | 883.5794   | 883.5802    | -0.90457   | 13  | 11469.54      | normal   | S1AcK5AcK8AcK12AcK16AcK20dMe  | 32  | 17      | 662.37  | S,0;K,0;K,0;K,0;K,0;K,16; | 1                |
| 1368           | 63.56    | 818.61     | 820.5383   | 820.5419    | -4.45066   | 14  | 11469.58      | normal   | R3dMeK5AcK8AcK12AcK16AcK20tMe | 15  | 10      | 361.46  | R,0;K,0;K,0;K,0;K,0;K,8;  | 1                |
| 1411           | 65.54    | 817.54     | 818.535    | 818.5397    | -5.68063   | 14  | 11441.55      | normal   | S1AcK5AcK8AcK16AcK20tMe       | 26  | 13      | 238.3   | S,2;K,2;K,1;K,7;K,1;      | 0                |
| 1423           | 66.08    | 883.78     | 883.5741   | 883.5802    | -6.91428   | 13  | 11469.54      | normal   | S1AcR3dMeK5AcK8AcK12AcK16Ac   | 25  | 18      | 372.85  | S,0;R,0;K,0;K,0;K,0;K,0;  | 1                |
| 1423           | 66.08    | 883.78     | 882.4972   | 882.5021    | -5.5361    | 13  | 11455.52      | normal   | S1AcR3MeK5AcK8AcK12AcK16Ac    | 27  | 15      | 435.05  | S,0;R,1;K,0;K,0;K,0;K,0;  | 1                |
| 1438           | 66.78    | 880.81     | 882.5009   | 882.5021    | -1.38641   | 13  | 11455.52      | normal   | S1AcK5AcK8AcK12AcK16AcK20Me   | 23  | 20      | 277.23  | S,0;K,0;K,0;K,0;K,0;K,2;  | 1                |
| 1438           | 66.78    | 880.81     | 876.965    | 876.9648    | 0.201628   | 13  | 11382.53      | A77→P    | R3MeK12AcK16AcK20dMe          | 20  | 19      | 295.69  | R,2;K,0;K,0;K,5;          | 1                |
| 1443           | 67.01    | 762.24     | 763.9009   | 763.9056    | -6.19199   | 15  | 11439.58      | A77→P    | R3dMeK8AcK12AcK16AcK20dMe     | 14  | 14      | 239.32  | R,4;K,1;K,0;K,0;K,3;      | 1                |
| 1444           | 67.05    | 762.24     | 763.9009   | 763.9032    | -3.01621   | 15  | 11439.54      | A77→P    | S1AcK8AcK12AcK16AcK20Me       | 37  | 5       | 287.24  | S,2;K,8;K,6;K,9;K,3;      | 0                |
| 1444           | 67.05    | 762.24     | 763.9009   | 763.9032    | -3.01621   | 15  | 11439.54      | A77→P    | S1AcK5AcK12AcK16AcK20Me       | 35  | 7       | 275.84  | S,2;K,1;K,6;K,9;K,3;      | 0                |
| 1444           | 67.05    | 762.24     | 762.17     | 762.1688    | 1.625552   | 15  | 11412.52      | normal   | S1AcK8AcK12AcK16AcK20Me       | 43  | 11      | 416.31  | S,2;K,8;K,6;K,9;K,3;      | 0                |
| 1444           | 67.05    | 762.24     | 762.17     | 762.1688    | 1.625552   | 15  | 11412.52      | normal   | S1AcK5AcK12AcK16AcK20Me       | 41  | 13      | 404.34  | S,2;K,1;K,6;K,9;K,3;      | 0                |
| 1444           | 67.05    | 762.24     | 762.9711   | 762.9688    | 2.967796   | 15  | 11424.52      | A77→P    | S1AcK8AcK12AcK16Ac            | 34  | 5       | 253.28  | S,2;K,8;K,6;K,6;          | 0                |
| 1445           | 67.09    | 816.54     | 813.2446   | 813.2471    | -3.06442   | 14  | 11366.45      | normal   | S1PR3MeK5Ac                   | 19  | 19      | 254.52  | S,1;R,0;K,0;              | 1                |
| 1462           | 67.88    | 818.04     | 819.2448   | 819.2512    | -7.76195   | 14  | 11450.51      | normal   | S1PR3MeK12AcK16AcK20tMe       | 20  | 14      | 278.9   | S,0;R,0;K,0;K,0;K,2;      | 1                |
| 1462           | 67.88    | 818.04     | 819.3923   | 819.3994    | -8.73085   | 14  | 11453.59      | A77→P    | R3dMeK8AcK12AcK16AcK20tMe     | 22  | 15      | 321.79  | R,2;K,0;K,0;K,0;K,8;      | 1                |
| 1463           | 67.92    | 818.04     | 819.3923   | 819.3968    | -5.55781   | 14  | 11453.55      | A77→P    | S1AcK8AcK12AcK16AcK20dMe      | 34  | 15      | 315.76  | S,2;K,7;K,7;K,13;K,8;     | 0                |
| 1463           | 67.92    | 818.04     | 819.3923   | 819.3968    | -5.55781   | 14  | 11453.55      | A77→P    | S1AcK5AcK12AcK16AcK20dMe      | 36  | 13      | 324.62  | S,2;K,3;K,7;K,13;K,8;     | 0                |
| 1463           | 67.92    | 818.04     | 819.3923   | 819.3968    | -5.55781   | 14  | 11453.55      | A77→P    | S1AcK5AcK8AcK16AcK20dMe       | 31  | 13      | 289.35  | S,2;K,3;K,2;K,13;K,8;     | 0                |
| 1478           | 68.61    | 818.68     | 814.2568   | 814.2482    | 10.63182   | 14  | 11380.47      | normal   | S1PK5AcK20dMe                 | 19  | 21      | 252.79  | S,1;K,0;K,1;              | 1                |
| 1478           | 68.61    | 818.68     | 816.5381   | 816.54      | -2.40045   | 14  | 11412.55      | normal   | R3MeK8AcK12AcK16AcK20tMe      | 27  | 27      | 544.04  | R,1;K,1;K,0;K,0;K,10;     | 1                |
| 1478           | 68.61    | 818.68     | 817.3964   | 817.3972    | -1.0126    | 14  | 11424.55      | A77→P    | S1AcR3MeK5AcK8AcK20dMe        | 18  | 21      | 300.32  | S,0;R,1;K,0;K,0;K,7;      | 1                |

|      |       |        |          |          |          |    |          |        |                              |    |    |         |                          |   |
|------|-------|--------|----------|----------|----------|----|----------|--------|------------------------------|----|----|---------|--------------------------|---|
| 1478 | 68.61 | 818.68 | 817.5387 | 817.5412 | -3.01968 | 14 | 11426.57 | normal | R3dMeK8AcK12AcK16AcK20tMe    | 45 | 22 | 1025.45 | R,4;K,3;K,0;K,0;K,24;    | 1 |
| 1487 | 69.03 | 951.46 | 954.7867 | 954.795  | -8.64147 | 12 | 11441.53 | normal | K5AcK8AcK12AcK16AcK20tMe     | 16 | 10 | 260.07  | K,0;K,0;K,0;K,0;K,1;     | 1 |
| 1505 | 69.86 | 764.1  | 762.9702 | 762.9688 | 1.847839 | 15 | 11424.52 | A77→P  | S1AcK5AcK12AcK16Ac           | 32 | 12 | 242.7   | S,2;K,3;K,7;K,8;         | 0 |
| 1520 | 70.55 | 817.54 | 815.5363 | 815.5389 | -3.20289 | 14 | 11398.54 | normal | K8AcK12AcK16AcK20tMe         | 28 | 24 | 645.88  | K,1;K,0;K,0;K,15;        | 1 |
| 1539 | 71.42 | 760.3  | 762.1689 | 762.1712 | -3.079   | 15 | 11412.56 | normal | R3dMeK5AcK8AcK12AcK20dMe     | 23 | 25 | 389.85  | R,5;K,3;K,1;K,2;K,4;     | 0 |
| 1542 | 71.56 | 814.47 | 819.1067 | 819.1072 | -0.61841 | 14 | 11448.49 | A77→P  | S1PR3MeK5AcK8AcK20Me         | 19 | 19 | 237.04  | S,1;R,0;K,0;K,0;K,4;     | 1 |
| 1542 | 71.56 | 814.47 | 813.2523 | 813.2497 | 3.194961 | 14 | 11366.49 | normal | R3dMeK20dMeY51P              | 30 | 20 | 401.94  | R,4;K,7;Y,5;             | 0 |
| 1542 | 71.56 | 814.47 | 813.2523 | 813.2471 | 6.392031 | 14 | 11366.45 | normal | S1AcK20MeY51P                | 31 | 31 | 401.94  | S,1;K,8;Y,5;             | 0 |
| 1542 | 71.56 | 814.47 | 811.3952 | 811.3957 | -0.58709 | 14 | 11340.53 | A77→P  | R3dMeK8AcK20Me               | 25 | 17 | 394.15  | R,4;K,1;K,6;             | 0 |
| 1542 | 71.56 | 814.47 | 811.3952 | 811.3957 | -0.58709 | 14 | 11340.53 | A77→P  | R3dMeK5AcK20Me               | 25 | 17 | 388.85  | R,4;K,2;K,6;             | 0 |
| 1542 | 71.56 | 814.47 | 816.3939 | 816.3987 | -5.81836 | 14 | 11410.57 | A77→P  | R3dMeK12AcK16AcK20tMe        | 33 | 27 | 476.94  | R,6;K,0;K,0;K,13;        | 2 |
| 1542 | 71.56 | 814.47 | 816.3939 | 816.3961 | -2.63365 | 14 | 11410.54 | A77→P  | S1AcR3MeK5AcK8AcK20Me        | 30 | 25 | 498.77  | S,0;R,0;K,0;K,0;K,15;    | 1 |
| 1542 | 71.56 | 814.47 | 816.5353 | 816.54   | -5.76413 | 14 | 11412.55 | normal | R3dMeK8AcK12AcK16AcK20dMe    | 31 | 25 | 466.06  | R,4;K,1;K,0;K,0;K,7;     | 1 |
| 1542 | 71.56 | 814.47 | 815.3938 | 815.3976 | -4.6041  | 14 | 11396.56 | A77→P  | R3MeK12AcK16AcK20tMe         | 22 | 18 | 305.16  | R,3;K,0;K,0;K,6;         | 1 |
| 1542 | 71.56 | 814.47 | 815.3938 | 815.3976 | -4.6041  | 14 | 11396.56 | A77→P  | R3dMeK12AcK16AcK20dMe        | 26 | 15 | 330.89  | R,7;K,0;K,0;K,4;         | 2 |
| 1542 | 71.56 | 814.47 | 817.3945 | 817.3972 | -3.2527  | 14 | 11424.55 | A77→P  | S1AcR3dMeK5AcK8AcK20Me       | 19 | 24 | 269.52  | S,0;R,2;K,0;K,0;K,2;     | 1 |
| 1542 | 71.56 | 814.47 | 815.5366 | 815.5389 | -2.90353 | 14 | 11398.54 | normal | R3dMeK8AcK12AcK16AcK20Me     | 30 | 23 | 468.88  | R,4;K,1;K,0;K,0;K,6;     | 1 |
| 1543 | 71.6  | 814.47 | 818.5383 | 818.5397 | -1.65407 | 14 | 11441.55 | normal | S1AcR3dMeK5AcK8AcK12AcK20Me  | 30 | 34 | 636.28  | S,0;R,0;K,0;K,0;K,0;K,7; | 2 |
| 1543 | 71.6  | 814.47 | 813.5353 | 813.5367 | -1.66144 | 14 | 11370.51 | normal | S1AcK5AcK8AcK20Me            | 35 | 45 | 576.64  | S,2;K,0;K,0;K,4;         | 1 |
| 1543 | 71.6  | 814.47 | 817.5373 | 817.5386 | -1.55653 | 14 | 11426.53 | normal | S1AcR3MeK5AcK8AcK12AcK20Me   | 31 | 39 | 630.91  | S,0;R,0;K,0;K,0;K,0;K,7; | 2 |
| 1544 | 71.65 | 877.12 | 878.0387 | 878.0401 | -1.61805 | 13 | 11396.51 | A77→P  | S1AcK5AcK8AcK20Me            | 22 | 22 | 287.69  | S,1;K,0;K,0;K,4;         | 1 |
| 1545 | 71.69 | 877.12 | 879.2712 | 879.2733 | -2.33689 | 13 | 11412.54 | normal | S1AcR3dMeK5AcK8AcK20dMe      | 27 | 53 | 490.87  | S,0;R,0;K,0;K,0;K,6;     | 1 |
| 1545 | 71.69 | 877.12 | 880.3481 | 880.3486 | -0.5435  | 13 | 11426.52 | normal | S1AcK5AcK8AcK12AcK20dMe      | 32 | 51 | 600.87  | S,2;K,0;K,0;K,0;K,7;     | 1 |
| 1545 | 71.69 | 877.12 | 880.3481 | 880.3486 | -0.5435  | 13 | 11426.52 | normal | S1AcR3dMeK5AcK8AcK12Ac       | 29 | 45 | 579.15  | S,0;R,2;K,0;K,0;K,0;     | 1 |
| 1547 | 71.79 | 712.85 | 714.4722 | 714.4725 | -0.43528 | 16 | 11410.55 | A77→P  | S1AcK12AcK16AcK20dMe         | 50 | 41 | 579.22  | S,2;K,6;K,24;K,22;       | 0 |
| 1548 | 71.83 | 950.13 | 954.7892 | 954.795  | -6.08448 | 12 | 11441.53 | normal | R3dMeK5AcK8AcK12AcK16AcK20Me | 33 | 31 | 498.91  | R,2;K,0;K,0;K,0;K,0;K,3; | 1 |
| 1548 | 71.83 | 950.13 | 948.6305 | 948.6233 | 7.58274  | 12 | 11366.47 | normal | S1PR3MeK20tMe                | 35 | 29 | 601.84  | S,1;R,0;K,1;             | 1 |

|      |       |        |          |          |          |    |          |        |                           |    |    |           |                       |   |
|------|-------|--------|----------|----------|----------|----|----------|--------|---------------------------|----|----|-----------|-----------------------|---|
| 1548 | 71.83 | 950.13 | 948.6305 | 948.6233 | 7.58274  | 12 | 11366.47 | normal | S1PR3dMeK20dMe            | 35 | 30 | 59<br>6.4 | S,1;R,0;K,7;          | 1 |
| 1548 | 71.83 | 950.13 | 952.2922 | 952.2941 | -1.97069 | 12 | 11410.52 | A77→P  | S1AcK5AcK8AcK20dMe        | 29 | 16 | 433.4     | S,1;K,0;K,0;K,16;     | 3 |
| 1548 | 71.83 | 950.13 | 952.2922 | 952.2941 | -1.97069 | 12 | 11410.52 | A77→P  | S1AcR3dMeK5AcK8Ac         | 28 | 16 | 430.8     | S,0;R,0;K,0;K,0;      | 1 |
| 1568 | 72.74 | 813.61 | 816.252  | 816.2478 | 5.143242 | 14 | 11408.46 | normal | S1PK12AcK16AcK20Me        | 26 | 18 | 298       | S,1;K,0;K,0;K,0;      | 1 |
| 1568 | 72.74 | 813.61 | 812.3957 | 812.3942 | 1.838908 | 14 | 11354.51 | A77→P  | K5AcK12AcK20Me            | 27 | 26 | 275.69    | K,2;K,1;K,3;          | 0 |
| 1568 | 72.74 | 813.61 | 813.3966 | 813.3953 | 1.586492 | 14 | 11368.53 | A77→P  | K5AcK12AcK20dMe           | 30 | 31 | 375.22    | K,2;K,1;K,6;          | 0 |
| 1568 | 72.74 | 813.61 | 814.5403 | 814.5404 | -0.15444 | 14 | 11384.56 | normal | R3dMeK12AcK16AcK20tMe     | 61 | 43 | 1313.02   | R,1;K,0;K,0;K,34;     | 1 |
| 1568 | 72.74 | 813.61 | 814.5403 | 814.5378 | 3.036327 | 14 | 11384.52 | normal | K5AcK12AcK16AcK20dMe      | 68 | 35 | 1411.62   | K,1;K,1;K,36;K,37;    | 0 |
| 1568 | 72.74 | 813.61 | 814.5403 | 814.5378 | 3.036327 | 14 | 11384.52 | normal | S1AcK12AcK16AcK20dMe      | 69 | 35 | 1420.91   | S,1;K,1;K,36;K,37;    | 0 |
| 1569 | 72.79 | 813.61 | 817.5519 | 817.5412 | 13.18089 | 14 | 11426.57 | normal | S1AcR3dMeK5AcK8AcK20tMe   | 16 | 47 | 348.96    | S,0;R,0;K,0;K,0;K,0;  | 1 |
| 1569 | 72.79 | 813.61 | 818.2433 | 818.2501 | -8.19533 | 14 | 11436.49 | normal | S1PR3MeK12AcK16AcK20dMe   | 16 | 52 | 359.07    | S,0;R,1;K,1;K,1;K,5;  | 1 |
| 1569 | 72.79 | 813.61 | 817.5349 | 817.5386 | -4.46816 | 14 | 11426.53 | normal | K5AcK8AcK12AcK16AcK20dMe  | 25 | 53 | 578.48    | K,3;K,2;K,1;K,8;K,11; | 1 |
| 1569 | 72.79 | 813.61 | 817.5349 | 817.5386 | -4.46816 | 14 | 11426.53 | normal | S1AcK5AcK12AcK16AcK20dMe  | 26 | 54 | 614.03    | S,2;K,1;K,1;K,8;K,11; | 0 |
| 1569 | 72.79 | 813.61 | 817.5349 | 817.5386 | -4.46816 | 14 | 11426.53 | normal | S1AcK5AcK8AcK16AcK20dMe   | 25 | 55 | 592.12    | S,2;K,1;K,2;K,8;K,11; | 0 |
| 1569 | 72.79 | 813.61 | 813.3966 | 813.3953 | 1.586492 | 14 | 11368.53 | A77→P  | S1AcK8AcK20dMe            | 23 | 25 | 349.32    | S,2;K,2;K,8;          | 0 |
| 1569 | 72.79 | 813.61 | 814.4007 | 814.3938 | 8.424426 | 14 | 11382.51 | A77→P  | K5AcK12AcK16Ac            | 20 | 46 | 279.15    | K,3;K,4;K,7;          | 0 |
| 1573 | 72.97 | 759.37 | 762.1692 | 762.1712 | -2.67859 | 15 | 11412.56 | normal | R3dMeK5AcK12AcK16AcK20dMe | 26 | 50 | 606.23    | R,3;K,3;K,1;K,5;K,9;  | 0 |
| 1573 | 72.97 | 759.37 | 762.1692 | 762.1712 | -2.67859 | 15 | 11412.56 | normal | R3dMeK5AcK8AcK16AcK20dMe  | 25 | 48 | 573.23    | R,3;K,3;K,2;K,5;K,8;  | 0 |
| 1573 | 72.97 | 759.37 | 761.2365 | 761.2369 | -0.45028 | 15 | 11398.54 | normal | R3MeK5AcK12AcK16AcK20dMe  | 32 | 49 | 771.93    | R,3;K,3;K,2;K,8;K,13; | 0 |
| 1573 | 72.97 | 759.37 | 761.2365 | 761.2369 | -0.45028 | 15 | 11398.54 | normal | R3MeK5AcK8AcK16AcK20dMe   | 30 | 47 | 695.52    | R,3;K,3;K,2;K,8;K,11; | 0 |
| 1573 | 72.97 | 759.37 | 760.1743 | 760.1705 | 4.984942 | 15 | 11382.55 | A77→P  | S1AcK12AcK20tMe           | 22 | 53 | 309.69    | S,2;K,7;K,3;          | 0 |
| 1573 | 72.97 | 759.37 | 760.1743 | 760.1705 | 4.984942 | 15 | 11382.55 | A77→P  | S1AcR3MeK5AcK20dMe        | 13 | 40 | 264.88    | S,0;R,1;K,2;K,6;      | 1 |
| 1578 | 73.2  | 810.46 | 812.5343 | 812.5356 | -1.56454 | 14 | 11356.49 | normal | K5AcK12AcK16Ac            | 35 | 42 | 549.32    | K,4;K,4;K,5;          | 0 |
| 1578 | 73.2  | 810.46 | 812.5343 | 812.5356 | -1.56454 | 14 | 11356.49 | normal | K5AcK8AcK16Ac             | 35 | 39 | 546.61    | K,4;K,3;K,5;          | 0 |
| 1578 | 73.2  | 810.46 | 814.5402 | 814.5378 | 2.961395 | 14 | 11384.52 | normal | S1AcK5AcK8AcK20dMe        | 65 | 55 | 1207.86   | S,2;K,0;K,0;K,38;     | 2 |
| 1578 | 73.2  | 810.46 | 814.5402 | 814.5378 | 2.961395 | 14 | 11384.52 | normal | S1AcR3dMeK5AcK8Ac         | 59 | 51 | 1138.97   | S,0;R,2;K,0;K,0;      | 1 |
| 1579 | 73.24 | 948.96 | 946.2893 | 946.2874 | 2.060305 | 12 | 11338.44 | normal | R3dMeS47P                 | 30 | 13 | 394.9     | R,2;S,1;              | 0 |

|      |       |        |          |          |          |    |          |        |                        |    |    |                        |                       |   |
|------|-------|--------|----------|----------|----------|----|----------|--------|------------------------|----|----|------------------------|-----------------------|---|
| 1579 | 73.24 | 948.96 | 948.9586 | 948.9612 | -2.78818 | 12 | 11370.53 | normal | R3dMeK12AcK16AcK20dMe  | 40 | 28 | 688.18                 | R,1;K,3;K,2;K,8;      | 4 |
| 1581 | 73.33 | 711.97 | 714.467  | 714.4748 | -10.8807 | 16 | 11410.59 | A77→P  | R3dMeK5AcK8AcK20tMe    | 19 | 19 | 327.59                 | R,3;K,2;K,1;K,1;      | 0 |
| 1582 | 73.38 | 711.97 | 714.467  | 714.4725 | -7.69657 | 16 | 11410.55 | A77→P  | S1AcK8AcK16AcK20dMe    | 47 | 28 | 512.66                 | S,2;K,4;K,26;K,21;    | 0 |
| 1584 | 73.47 | 815.03 | 812.5343 | 812.5382 | -4.76315 | 14 | 11356.53 | normal | R3MeK8AcK16AcK20dMe    | 29 | 43 | 557.99                 | R,1;K,2;K,5;K,7;      | 0 |
| 1584 | 73.47 | 815.03 | 811.5395 | 811.5371 | 3.001398 | 14 | 11342.51 | normal | K8AcK16AcK20dMe        | 34 | 43 | 569                    | K,4;K,4;K,6;          | 0 |
| 1584 | 73.47 | 815.03 | 811.5395 | 811.5371 | 3.001398 | 14 | 11342.51 | normal | K8AcK12AcK20dMe        | 33 | 43 | 461.59                 | K,4;K,4;K,1;          | 0 |
| 1584 | 73.47 | 815.03 | 813.5406 | 813.5393 | 1.594734 | 14 | 11370.54 | normal | R3dMeK8AcK16AcK20dMe   | 29 | 41 | 520.04                 | R,1;K,2;K,4;K,6;      | 0 |
| 1584 | 73.47 | 815.03 | 814.5402 | 814.5378 | 2.961395 | 14 | 11384.52 | normal | K5AcK8AcK16AcK20dMe    | 71 | 68 | <sup>12</sup><br>87.88 | K,3;K,3;K,36;K,34;    | 0 |
| 1584 | 73.47 | 815.03 | 814.5402 | 814.5378 | 2.961395 | 14 | 11384.52 | normal | S1AcK8AcK16AcK20dMe    | 75 | 68 | 1378.93                | S,2;K,3;K,36;K,35;    | 0 |
| 1584 | 73.47 | 815.03 | 814.5402 | 814.5378 | 2.961395 | 14 | 11384.52 | normal | S1AcR3MeK5AcK8AcK20Me  | 61 | 64 | 1209.6                 | S,0;R,2;K,2;K,2;K,33; | 1 |
| 1588 | 73.65 | 877.65 | 882.1889 | 882.193  | -4.60692 | 13 | 11450.5  | normal | S1PR3dMeK5AcK8AcK20dMe | 25 | 20 | 316.91                 | S,1;R,0;K,0;K,0;K,2;  | 1 |
| 1589 | 73.7  | 877.65 | 882.1889 | 882.1902 | -1.43301 | 13 | 11450.46 | normal | S1PR3MeK5AcK8AcK12Ac   | 18 | 29 | 262.62                 | S,1;R,0;K,0;K,0;K,0;  | 1 |
| 1591 | 73.79 | 811.54 | 816.2472 | 816.2478 | -0.764   | 14 | 11408.46 | normal | S1PK5AcK8AcK20Me       | 23 | 40 | 436.21                 | S,0;K,0;K,0;K,2;      | 1 |
| 1591 | 73.79 | 811.54 | 816.2472 | 816.2478 | -0.764   | 14 | 11408.46 | normal | S1PR3MeK5AcK8Ac        | 24 | 36 | 438.83                 | S,1;R,0;K,0;K,0;      | 1 |
| 1591 | 73.79 | 811.54 | 815.5368 | 815.5389 | -2.60417 | 14 | 11398.54 | normal | S1AcK12AcK16AcK20tMe   | 41 | 35 | 685.28                 | S,2;K,3;K,7;K,5;      | 0 |
| 1591 | 73.79 | 811.54 | 815.5368 | 815.5389 | -2.60417 | 14 | 11398.54 | normal | S1AcK8AcK16AcK20tMe    | 41 | 35 | 682.5                  | S,2;K,4;K,7;K,5;      | 0 |
| 1591 | 73.79 | 811.54 | 815.5368 | 815.5363 | 0.583909 | 14 | 11398.5  | normal | S1AcK5AcK8AcK12Ac      | 30 | 34 | 618.91                 | S,2;K,0;K,0;K,0;      | 1 |
| 1597 | 74.07 | 950.63 | 953.2836 | 953.2891 | -5.82264 | 12 | 11422.46 | normal | S1PK12AcK16AcK20dMe    | 32 | 17 | 532.66                 | S,0;K,1;K,1;K,4;      | 1 |
| 1597 | 74.07 | 950.63 | 953.2836 | 953.2891 | -5.82264 | 12 | 11422.46 | normal | S1PR3MeK5AcK8AcK20Me   | 31 | 15 | 502.82                 | S,0;R,0;K,0;K,0;K,3;  | 1 |
| 1597 | 74.07 | 950.63 | 947.4551 | 947.4553 | -0.20037 | 12 | 11352.46 | normal | S1PR3MeK20dMe          | 32 | 19 | 525.11                 | S,0;R,0;K,4;          | 1 |
| 1597 | 74.07 | 950.63 | 947.4551 | 947.4553 | -0.20037 | 12 | 11352.46 | normal | S1PR3dMeK20Me          | 33 | 17 | 568.88                 | S,0;R,0;K,5;          | 2 |
| 1597 | 74.07 | 950.63 | 950.9565 | 950.9562 | 0.285958 | 12 | 11394.47 | normal | S1PR3MeK16AcK20dMe     | 34 | 17 | 609.9                  | S,0;R,0;K,1;K,6;      | 1 |
| 1601 | 74.25 | 815.75 | 818.2468 | 818.2501 | -4.01816 | 14 | 11436.49 | normal | S1PK12AcK16AcK20tMe    | 26 | 25 | 366.47                 | S,1;K,0;K,1;K,3;      | 1 |
| 1601 | 74.25 | 815.75 | 812.2544 | 812.2485 | 7.205345 | 14 | 11352.47 | normal | K20tMeS47P             | 23 | 30 | 259.87                 | K,2;S,1;              | 0 |
| 1601 | 74.25 | 815.75 | 812.2544 | 812.2485 | 7.205345 | 14 | 11352.47 | normal | R3dMeK20MeS47P         | 23 | 34 | 262.36                 | R,1;K,2;S,1;          | 0 |
| 1601 | 74.25 | 815.75 | 813.5397 | 813.5393 | 0.544395 | 14 | 11370.54 | normal | R3MeK12AcK16AcK20tMe   | 39 | 27 | 729.5                  | R,3;K,0;K,14;K,14;    | 1 |
| 1602 | 74.29 | 815.75 | 818.2468 | 818.2501 | -4.01816 | 14 | 11436.49 | normal | S1PK5AcK8AcK20tMe      | 29 | 18 | 455.8                  | S,3;K,0;K,0;K,0;      | 2 |

|      |       |        |          |          |          |    |          |        |                          |    |    |        |                      |   |
|------|-------|--------|----------|----------|----------|----|----------|--------|--------------------------|----|----|--------|----------------------|---|
| 1602 | 74.29 | 815.75 | 818.2468 | 818.2501 | -4.01816 | 14 | 11436.49 | normal | S1PR3MeK5AcK8AcK20dMe    | 29 | 24 | 484.95 | S,2;R,0;K,0;K,2;     | 1 |
| 1602 | 74.29 | 815.75 | 811.2394 | 811.2474 | -9.83927 | 14 | 11338.46 | normal | S1PR3MeK20Me             | 32 | 34 | 550.29 | S,2;R,0;K,5;         | 3 |
| 1602 | 74.29 | 815.75 | 811.2394 | 811.2474 | -9.83927 | 14 | 11338.46 | normal | S1PR3dMe                 | 30 | 34 | 520.58 | S,1;R,0;             | 1 |
| 1602 | 74.29 | 815.75 | 815.5329 | 815.5389 | -7.39395 | 14 | 11398.54 | normal | S1AcR3MeK5AcK8AcK20dMe   | 32 | 33 | 598.79 | S,0;R,0;K,0;K,4;     | 2 |
| 1602 | 74.29 | 815.75 | 815.5329 | 815.5389 | -7.39395 | 14 | 11398.54 | normal | S1AcR3dMeK5AcK8AcK20Me   | 32 | 29 | 629.03 | S,0;R,0;K,0;K,0;K,5; | 1 |
| 1602 | 74.29 | 815.75 | 812.5361 | 812.5382 | -2.50965 | 14 | 11356.53 | normal | S1AcK8AcK20tMe           | 40 | 35 | 596.46 | S,2;K,5;K,2;         | 0 |
| 1602 | 74.29 | 815.75 | 812.5361 | 812.5356 | 0.68897  | 14 | 11356.49 | normal | S1AcK12AcK16Ac           | 43 | 39 | 634.98 | S,2;K,3;K,6;         | 0 |
| 1602 | 74.29 | 815.75 | 813.5397 | 813.5367 | 3.740319 | 14 | 11370.51 | normal | S1AcR3MeK5AcK8Ac         | 36 | 38 | 560.85 | S,0;R,0;K,0;K,0;     | 2 |
| 1608 | 74.57 | 878.35 | 880.0396 | 880.0367 | 3.293972 | 13 | 11422.47 | normal | S1PK5AcK8AcK20dMe        | 28 | 17 | 375.52 | S,2;K,0;K,0;K,3;     | 1 |
| 1608 | 74.57 | 878.35 | 880.0396 | 880.0367 | 3.293972 | 13 | 11422.47 | normal | S1PR3MeK12AcK16AcK20Me   | 27 | 18 | 346.84 | S,2;R,0;K,0;K,0;K,2; | 1 |
| 1608 | 74.57 | 878.35 | 880.0396 | 880.0367 | 3.293972 | 13 | 11422.47 | normal | S1PR3dMeK5AcK8Ac         | 28 | 17 | 386.02 | S,2;R,0;K,0;K,0;     | 1 |
| 1608 | 74.57 | 878.35 | 881.1125 | 881.1148 | -2.60031 | 13 | 11436.48 | normal | S1PR3dMeK5AcK8AcK20Me    | 25 | 19 | 310.73 | S,1;R,0;K,0;K,0;K,0; | 1 |
| 1608 | 74.57 | 878.35 | 881.4185 | 881.424  | -6.23193 | 13 | 11440.5  | normal | S1AcK5AcK8AcK12AcK16Ac   | 30 | 20 | 460.5  | S,0;K,0;K,0;K,0;K,0; | 1 |
| 1608 | 74.57 | 878.35 | 875.8875 | 875.8895 | -2.29461 | 13 | 11368.55 | A77→P  | R3dMeK5AcK20tMe          | 36 | 19 | 731.5  | R,4;K,2;K,18;        | 0 |
| 1608 | 74.57 | 878.35 | 875.8875 | 875.8867 | 0.900998 | 13 | 11368.52 | A77→P  | S1AcK5AcK20dMe           | 33 | 17 | 632.07 | S,0;K,2;K,14;        | 1 |
| 1609 | 74.61 | 878.35 | 881.1125 | 881.112  | 0.577484 | 13 | 11436.45 | normal | S1PK5AcK8AcK12Ac         | 19 | 15 | 310.48 | S,1;K,0;K,0;K,0;     | 1 |
| 1609 | 74.61 | 878.35 | 881.4185 | 881.4268 | -9.40857 | 13 | 11441.54 | normal | S1AcK8AcK12AcK16AcK20tMe | 28 | 22 | 435.28 | S,2;K,3;K,1;K,2;K,3; | 0 |
| 1609 | 74.61 | 878.35 | 881.4185 | 881.4268 | -9.40857 | 13 | 11441.54 | normal | S1AcK5AcK12AcK16AcK20tMe | 27 | 23 | 429.97 | S,2;K,2;K,1;K,2;K,3; | 0 |
| 1609 | 74.61 | 878.35 | 878.1937 | 878.1952 | -1.64134 | 13 | 11398.53 | normal | K5AcK12AcK16AcK20tMe     | 38 | 33 | 582.22 | K,3;K,6;K,11;K,5;    | 0 |
| 1609 | 74.61 | 878.35 | 878.1937 | 878.1952 | -1.64134 | 13 | 11398.53 | normal | K5AcK8AcK16AcK20tMe      | 40 | 32 | 598.85 | K,3;K,3;K,11;K,5;    | 0 |
| 1609 | 74.61 | 878.35 | 878.1937 | 878.1952 | -1.64134 | 13 | 11398.53 | normal | K5AcK8AcK12AcK20tMe      | 35 | 31 | 554.65 | K,3;K,3;K,1;K,5;     | 0 |
| 1609 | 74.61 | 878.35 | 878.1937 | 878.1952 | -1.64134 | 13 | 11398.53 | normal | S1AcK8AcK12AcK20tMe      | 36 | 27 | 532.72 | S,2;K,3;K,1;K,4;     | 0 |
| 1609 | 74.61 | 878.35 | 878.1937 | 878.1952 | -1.64134 | 13 | 11398.53 | normal | S1AcK5AcK16AcK20tMe      | 40 | 29 | 571.17 | S,2;K,1;K,11;K,4;    | 0 |
| 1609 | 74.61 | 878.35 | 878.1937 | 878.1952 | -1.64134 | 13 | 11398.53 | normal | S1AcK5AcK12AcK20tMe      | 35 | 28 | 527.26 | S,2;K,1;K,1;K,4;     | 0 |
| 1609 | 74.61 | 878.35 | 878.1937 | 878.1924 | 1.547025 | 13 | 11398.49 | normal | K5AcK8AcK12AcK16Ac       | 29 | 30 | 508.19 | K,3;K,3;K,1;K,5;     | 0 |
| 1609 | 74.61 | 878.35 | 876.0413 | 876.0389 | 2.74965  | 13 | 11370.5  | normal | S1AcK5AcK12AcK20Me       | 39 | 30 | 470.58 | S,2;K,1;K,1;K,4;     | 0 |
| 1609 | 74.61 | 878.35 | 877.1188 | 877.117  | 1.977403 | 13 | 11384.51 | normal | S1AcK8AcK12AcK20dMe      | 58 | 48 | 887.19 | S,2;K,3;K,1;K,22;    | 0 |

|      |       |        |          |          |          |    |          |        |                             |    |    |        |                      |   |
|------|-------|--------|----------|----------|----------|----|----------|--------|-----------------------------|----|----|--------|----------------------|---|
| 1609 | 74.61 | 878.35 | 877.1188 | 877.117  | 1.977403 | 13 | 11384.51 | normal | S1AcK5AcK16AcK20dMe         | 62 | 51 | 928.21 | S,2;K,2;K,29;K,22;   | 0 |
| 1609 | 74.61 | 878.35 | 877.1188 | 877.117  | 1.977403 | 13 | 11384.51 | normal | S1AcK5AcK12AcK20dMe         | 57 | 49 | 881.34 | S,2;K,2;K,1;K,22;    | 0 |
| 1611 | 74.7  | 713.72 | 713.5929 | 713.5966 | -5.13664 | 16 | 11396.54 | A77→P  | S1AcK12AcK16AcK20Me         | 33 | 18 | 250.43 | S,2;K,6;K,9;K,2;     | 0 |
| 1611 | 74.7  | 713.72 | 713.5929 | 713.5966 | -5.13664 | 16 | 11396.54 | A77→P  | S1AcK8AcK16AcK20Me          | 38 | 17 | 287.73 | S,2;K,8;K,9;K,2;     | 0 |
| 1611 | 74.7  | 713.72 | 713.5929 | 713.5966 | -5.13664 | 16 | 11396.54 | A77→P  | S1AcK5AcK16AcK20Me          | 37 | 17 | 279.68 | S,2;K,1;K,9;K,2;     | 0 |
| 1616 | 74.94 | 760.83 | 762.972  | 762.9688 | 4.247747 | 15 | 11424.52 | A77→P  | K5AcK8AcK12AcK16Ac          | 15 | 13 | 235.63 | K,0;K,0;K,0;K,0;     | 1 |
| 1616 | 74.94 | 760.83 | 759.2382 | 759.2386 | -0.549   | 15 | 11368.57 | A77→P  | R3dMeK8AcK20tMe             | 19 | 13 | 354.88 | R,4;K,1;K,8;         | 0 |
| 1617 | 74.98 | 760.83 | 763.1042 | 763.1032 | 1.396989 | 15 | 11426.54 | normal | S1AcK8AcK12AcK16AcK20dMe    | 39 | 29 | 610.38 | S,2;K,6;K,1;K,4;K,5; | 0 |
| 1617 | 74.98 | 760.83 | 759.3712 | 759.3705 | 0.908411 | 15 | 11370.55 | normal | S1AcR3dMeK16AcK20dMe        | 40 | 31 | 641.79 | S,1;R,1;K,8;K,8;     | 0 |
| 1617 | 74.98 | 760.83 | 759.3712 | 759.3681 | 4.103175 | 15 | 11370.51 | normal | K5AcK12AcK16AcK20Me         | 52 | 41 | 735.51 | K,2;K,5;K,12;K,8;    | 0 |
| 1617 | 74.98 | 760.83 | 759.3712 | 759.3681 | 4.103175 | 15 | 11370.51 | normal | K5AcK8AcK16AcK20Me          | 54 | 41 | 746.98 | K,2;K,6;K,12;K,8;    | 0 |
| 1617 | 74.98 | 760.83 | 759.3712 | 759.3681 | 4.103175 | 15 | 11370.51 | normal | S1AcK12AcK16AcK20Me         | 55 | 39 | 790.19 | S,2;K,5;K,12;K,8;    | 0 |
| 1617 | 74.98 | 760.83 | 759.3712 | 759.3681 | 4.103175 | 15 | 11370.51 | normal | S1AcK8AcK16AcK20Me          | 57 | 39 | 807.55 | S,2;K,6;K,12;K,8;    | 0 |
| 1622 | 75.21 | 758.5  | 763.0983 | 763.1032 | -6.44133 | 15 | 11426.54 | normal | R3MeK5AcK8AcK12AcK16AcK20Me | 22 | 35 | 293.45 | R,2;K,0;K,0;K,0;K,1; | 1 |
| 1622 | 75.21 | 758.5  | 761.2333 | 761.2369 | -4.69976 | 15 | 11398.54 | normal | S1AcK5AcK8AcK20tMe          | 32 | 34 | 410.58 | S,2;K,2;K,1;K,3;     | 0 |
| 1623 | 75.26 | 875.04 | 874.8075 | 874.8085 | -1.18755 | 13 | 11354.5  | A77→P  | S1AcK12AcK20Me              | 26 | 19 | 338.14 | S,1;K,1;K,6;         | 0 |
| 1623 | 75.26 | 875.04 | 875.8862 | 875.8867 | -0.56236 | 13 | 11368.52 | A77→P  | R3MeK12AcK16AcK20Me         | 29 | 19 | 489.04 | R,3;K,0;K,0;K,11;    | 1 |
| 1623 | 75.26 | 875.04 | 875.8862 | 875.8867 | -0.56236 | 13 | 11368.52 | A77→P  | S1AcK12AcK20dMe             | 32 | 21 | 508.07 | S,1;K,1;K,12;        | 0 |
| 1623 | 75.26 | 875.04 | 876.9655 | 876.962  | 3.951256 | 13 | 11382.5  | A77→P  | S1AcK12AcK16Ac              | 27 | 27 | 314.89 | S,1;K,1;K,5;         | 0 |
| 1624 | 75.3  | 875.04 | 879.2688 | 879.2705 | -1.92907 | 13 | 11412.51 | normal | S1AcK5AcK8AcK16AcK20Me      | 21 | 31 | 296.93 | S,2;K,2;K,1;K,3;K,3; | 0 |
| 1624 | 75.3  | 875.04 | 878.1934 | 878.1924 | 1.199521 | 13 | 11398.49 | normal | S1AcK5AcK8AcK16Ac           | 21 | 30 | 297    | S,2;K,2;K,1;K,3;     | 0 |
| 1627 | 75.44 | 951.46 | 947.4437 | 947.4553 | -12.2469 | 12 | 11352.46 | normal | S1PK20tMe                   | 28 | 15 | 453.36 | S,0;K,1;             | 1 |
| 1636 | 75.85 | 872.65 | 875.8851 | 875.8867 | -1.81667 | 13 | 11368.52 | A77→P  | R3dMeK5AcK8Ac               | 23 | 17 | 353.12 | R,4;K,2;K,1;         | 0 |
| 1641 | 76.09 | 760.24 | 762.0432 | 762.0369 | 8.26319  | 15 | 11410.54 | A77→P  | R3dMeK8AcK12AcK16Ac         | 19 | 22 | 274.95 | R,3;K,0;K,0;K,0;     | 1 |
| 1642 | 76.13 | 760.24 | 762.1594 | 762.1688 | -12.3085 | 15 | 11412.52 | normal | K5AcK8AcK12AcK16AcK20Me     | 33 | 46 | 426.82 | K,3;K,7;K,3;K,1;K,1; | 0 |
| 1642 | 76.13 | 760.24 | 762.1594 | 762.1688 | -12.3085 | 15 | 11412.52 | normal | R3MeK5AcK8AcK12AcK16Ac      | 24 | 46 | 350.65 | R,4;K,0;K,0;K,0;K,1; | 1 |
| 1642 | 76.13 | 760.24 | 761.2338 | 761.2344 | -0.79124 | 15 | 11398.51 | normal | S1AcK8AcK12AcK16Ac          | 39 | 43 | 535.09 | S,2;K,7;K,2;K,5;     | 0 |

|      |       |        |          |          |          |    |          |        |                      |    |    |                               |                   |   |
|------|-------|--------|----------|----------|----------|----|----------|--------|----------------------|----|----|-------------------------------|-------------------|---|
| 1644 | 76.22 | 761.37 | 762.0432 | 762.0369 | 8.26319  | 15 | 11410.54 | A77→P  | S1AcK8AcK12AcK20dMe  | 38 | 20 | 327.04                        | S,2;K,6;K,2;K,12; | 0 |
| 1644 | 76.22 | 761.37 | 758.4359 | 758.4337 | 2.808486 | 15 | 11356.5  | normal | S1AcK8AcK16Ac        | 49 | 43 | 635.25                        | S,2;K,6;K,14;     | 0 |
| 1646 | 76.31 | 711.35 | 714.4707 | 714.4725 | -2.57095 | 16 | 11410.55 | A77→P  | S1AcK5AcK16AcK20dMe  | 36 | 19 | 304.51                        | S,2;K,1;K,10;K,7; | 0 |
| 1646 | 76.31 | 711.35 | 714.4707 | 714.4725 | -2.57095 | 16 | 11410.55 | A77→P  | S1AcK5AcK12AcK20dMe  | 34 | 17 | 293.47                        | S,2;K,1;K,2;K,7;  | 0 |
| 1646 | 76.31 | 711.35 | 712.7235 | 712.7206 | 4.10784  | 16 | 11382.52 | A77→P  | S1AcK5AcK8Ac         | 27 | 9  | 244.62                        | S,2;K,1;K,1;      | 1 |
| 1652 | 76.59 | 877.12 | 874.9626 | 874.9636 | -1.07149 | 13 | 11356.52 | normal | R3MeK12AcK16AcK20dMe | 34 | 29 | <sup>66</sup> <sub>3.89</sub> | R,1;K,0;K,0;K,13; | 1 |
| 1654 | 76.68 | 814.47 | 814.3964 | 814.3964 | -0.01309 | 14 | 11382.54 | A77→P  | K12AcK16AcK20tMe     | 23 | 28 | 322.49                        | K,0;K,0;K,9;      | 1 |
| 1654 | 76.68 | 814.47 | 814.3964 | 814.3964 | -0.01309 | 14 | 11382.54 | A77→P  | R3dMeK12AcK16AcK20Me | 25 | 26 | 340.69                        | R,5;K,0;K,0;K,7;  | 2 |
| 1654 | 76.68 | 814.47 | 812.5375 | 812.5382 | -0.85708 | 14 | 11356.53 | normal | K12AcK16AcK20tMe     | 41 | 28 | 862                           | K,0;K,0;K,19;     | 1 |
| 1654 | 76.68 | 814.47 | 812.5375 | 812.5382 | -0.85708 | 14 | 11356.53 | normal | R3dMeK12AcK16AcK20Me | 42 | 25 | 870.86                        | R,3;K,0;K,0;K,18; | 1 |
| 1657 | 76.82 | 712.85 | 712.7222 | 712.7229 | -0.88112 | 16 | 11382.56 | A77→P  | S1AcK8AcK20tMe       | 32 | 9  | 237.5                         | S,2;K,8;K,2;      | 0 |
| 1657 | 76.82 | 712.85 | 712.7222 | 712.7206 | 2.309466 | 16 | 11382.52 | A77→P  | S1AcK8AcK16Ac        | 41 | 12 | 339.34                        | S,2;K,8;K,11;     | 0 |
| 1657 | 76.82 | 712.85 | 712.7222 | 712.7206 | 2.309466 | 16 | 11382.52 | A77→P  | S1AcK8AcK12Ac        | 41 | 10 | 339.34                        | S,2;K,8;K,3;      | 0 |
| 1657 | 76.82 | 712.85 | 712.7222 | 712.7206 | 2.309466 | 16 | 11382.52 | A77→P  | S1AcK5AcK16Ac        | 39 | 13 | 325.3                         | S,2;K,1;K,11;     | 0 |
| 1657 | 76.82 | 712.85 | 712.7222 | 712.7206 | 2.309466 | 16 | 11382.52 | A77→P  | S1AcK5AcK12Ac        | 39 | 11 | 325.3                         | S,2;K,1;K,3;      | 0 |
| 1671 | 77.46 | 812.97 | 812.3954 | 812.3942 | 1.463258 | 14 | 11354.51 | A77→P  | S1AcK5AcK20Me        | 22 | 26 | 306.39                        | S,1;K,2;K,6;      | 1 |
| 1671 | 77.46 | 812.97 | 814.3961 | 814.3964 | -0.38782 | 14 | 11382.54 | A77→P  | S1AcK5AcK20tMe       | 23 | 39 | 271.23                        | S,1;K,2;K,1;      | 0 |
| 1671 | 77.46 | 812.97 | 812.5377 | 812.5382 | -0.63173 | 14 | 11356.53 | normal | S1AcK5AcK20tMe       | 40 | 41 | 764.46                        | S,1;K,2;K,17;     | 0 |
| 1672 | 77.51 | 812.97 | 815.5352 | 815.5363 | -1.43678 | 14 | 11398.5  | normal | S1AcK5AcK12AcK16Ac   | 26 | 40 | 491.78                        | S,2;K,1;K,3;K,6;  | 0 |
| 1672 | 77.51 | 812.97 | 812.5377 | 812.5356 | 2.566892 | 14 | 11356.49 | normal | S1AcK8AcK12Ac        | 37 | 56 | 605.24                        | S,2;K,2;K,3;      | 0 |
| 1672 | 77.51 | 812.97 | 812.5377 | 812.5356 | 2.566892 | 14 | 11356.49 | normal | S1AcK5AcK12Ac        | 37 | 57 | 605.24                        | S,2;K,3;K,3;      | 0 |
| 1672 | 77.51 | 812.97 | 812.5377 | 812.5356 | 2.566892 | 14 | 11356.49 | normal | S1AcK5AcK8Ac         | 36 | 54 | 627.13                        | S,2;K,3;K,0;      | 1 |
| 1672 | 77.51 | 812.97 | 814.5378 | 814.5378 | -0.0359  | 14 | 11384.52 | normal | K5AcK8AcK12AcK20dMe  | 35 | 54 | 613.15                        | K,3;K,2;K,3;K,10; | 0 |
| 1674 | 77.6  | 813.54 | 811.3967 | 811.3931 | 4.497839 | 14 | 11340.49 | A77→P  | K5AcK16Ac            | 22 | 36 | 372.89                        | K,2;K,7;          | 0 |
| 1674 | 77.6  | 813.54 | 814.3951 | 814.3964 | -1.58694 | 14 | 11382.54 | A77→P  | K5AcK16AcK20tMe      | 20 | 34 | 247.12                        | K,2;K,6;K,7;      | 0 |
| 1674 | 77.6  | 813.54 | 814.3951 | 814.3964 | -1.58694 | 14 | 11382.54 | A77→P  | S1AcK16AcK20tMe      | 22 | 34 | 259.32                        | S,1;K,7;K,8;      | 0 |
| 1675 | 77.64 | 813.54 | 813.538  | 813.5393 | -1.55628 | 14 | 11370.54 | normal | R3dMeK5AcK16AcK20dMe | 28 | 35 | 607.5                         | R,3;K,2;K,6;K,11; | 0 |

|      |       |        |          |          |          |    |          |        |                        |    |    |         |                      |   |
|------|-------|--------|----------|----------|----------|----|----------|--------|------------------------|----|----|---------|----------------------|---|
| 1675 | 77.64 | 813.54 | 812.5381 | 812.5382 | -0.10592 | 14 | 11356.53 | normal | K8AcK16AcK20tMe        | 34 | 44 | 594.01  | K,4;K,12;K,15;       | 0 |
| 1676 | 77.69 | 873.89 | 874.8097 | 874.8113 | -1.87654 | 13 | 11354.54 | A77→P  | R3dMeK5AcK20dMe        | 27 | 22 | 390.14  | R,5;K,3;K,6;         | 0 |
| 1676 | 77.69 | 873.89 | 874.8097 | 874.8085 | 1.324156 | 13 | 11354.5  | A77→P  | K12AcK16AcK20Me        | 28 | 23 | 426.35  | K,1;K,8;K,8;         | 1 |
| 1679 | 77.83 | 759.24 | 757.3699 | 757.3698 | 0.149309 | 15 | 11340.54 | A77→P  | S1AcR3MeK20dMe         | 13 | 47 | 233.63  | S,0;R,2;K,6;         | 1 |
| 1681 | 77.92 | 710.22 | 714.5965 | 714.5962 | 0.354861 | 16 | 11412.53 | normal | S1AcK5AcK8AcK12AcK20Me | 31 | 52 | 687.12  | S,2;K,0;K,0;K,0;K,8; | 1 |
| 1681 | 77.92 | 710.22 | 714.5965 | 714.5962 | 0.354861 | 16 | 11412.53 | normal | S1AcR3MeK5AcK8AcK12Ac  | 31 | 50 | 692.75  | S,0;R,2;K,0;K,0;K,0; | 2 |
| 1681 | 77.92 | 710.22 | 711.8456 | 711.8469 | -1.73761 | 16 | 11368.54 | A77→P  | K12AcK16AcK20dMe       | 45 | 63 | 749.91  | K,3;K,34;K,30;       | 1 |
| 1681 | 77.92 | 710.22 | 711.8456 | 711.8469 | -1.73761 | 16 | 11368.54 | A77→P  | K5AcK16AcK20dMe        | 49 | 66 | 778.46  | K,2;K,34;K,30;       | 0 |
| 1681 | 77.92 | 710.22 | 711.8456 | 711.8469 | -1.73761 | 16 | 11368.54 | A77→P  | S1AcK16AcK20dMe        | 50 | 66 | 741.37  | S,2;K,34;K,30;       | 0 |
| 1681 | 77.92 | 710.22 | 710.097  | 710.0949 | 2.991006 | 16 | 11340.51 | A77→P  | K12AcK16Ac             | 26 | 48 | 399.01  | K,4;K,13;            | 0 |
| 1681 | 77.92 | 710.22 | 711.9715 | 711.9729 | -1.91077 | 16 | 11370.56 | normal | R3dMeK5AcK8AcK20dMe    | 26 | 64 | 556.98  | R,2;K,1;K,2;K,5;     | 0 |
| 1681 | 77.92 | 710.22 | 710.2222 | 710.2209 | 1.871254 | 16 | 11342.53 | normal | K12AcK16AcK20dMe       | 69 | 82 | 1297.54 | K,3;K,36;K,32;       | 2 |
| 1681 | 77.92 | 710.22 | 710.2222 | 710.2209 | 1.871254 | 16 | 11342.53 | normal | K5AcK16AcK20dMe        | 74 | 90 | 1401.81 | K,2;K,36;K,34;       | 0 |
| 1681 | 77.92 | 710.22 | 711.0963 | 711.0969 | -0.79388 | 16 | 11356.54 | normal | K5AcK16AcK20tMe        | 41 | 71 | 778.61  | K,4;K,10;K,9;        | 0 |
| 1681 | 77.92 | 710.22 | 711.0963 | 711.0969 | -0.79388 | 16 | 11356.54 | normal | R3MeK5AcK16AcK20dMe    | 33 | 70 | 798.68  | R,4;K,3;K,7;K,9;     | 0 |
| 1681 | 77.92 | 710.22 | 711.0963 | 711.0969 | -0.79388 | 16 | 11356.54 | normal | S1AcK16AcK20tMe        | 40 | 69 | 654.04  | S,2;K,10;K,6;        | 0 |
| 1681 | 77.92 | 710.22 | 711.0963 | 711.0969 | -0.79388 | 16 | 11356.54 | normal | S1AcR3dMeK5AcK20Me     | 30 | 66 | 656.84  | S,0;R,0;K,0;K,9;     | 1 |
| 1687 | 78.17 | 946.62 | 945.4555 | 945.4603 | -5.09342 | 12 | 11328.52 | normal | R3dMeK16AcK20dMe       | 44 | 31 | 752.32  | R,3;K,3;K,10;        | 2 |
| 1688 | 78.22 | 946.62 | 946.6248 | 946.6253 | -0.53257 | 12 | 11342.49 | normal | S1AcR3MeK12AcK20Me     | 48 | 49 | 780.1   | S,1;R,3;K,1;K,28;    | 0 |
| 1693 | 78.44 | 1032.5 | 1030.941 | 1030.948 | -6.35133 | 11 | 11324.42 | normal | S1PK20Me               | 33 | 23 | 626.02  | S,0;K,8;             | 3 |
| 1709 | 79.15 | 947.13 | 949.7914 | 949.7882 | 3.373248 | 12 | 11380.45 | normal | S1PK16AcK20dMe         | 38 | 26 | 604.73  | S,1;K,1;K,6;         | 1 |
| 1709 | 79.15 | 947.13 | 949.7914 | 949.7882 | 3.373248 | 12 | 11380.45 | normal | S1PK12AcK20dMe         | 38 | 25 | 594.07  | S,1;K,4;K,6;         | 0 |
| 1710 | 79.2  | 947.13 | 947.776  | 947.7902 | -14.9791 | 12 | 11356.47 | normal | K8AcK12AcK16Ac         | 17 | 30 | 321.42  | K,4;K,0;K,0;         | 2 |
| 1711 | 79.24 | 810.4  | 814.2462 | 814.2482 | -2.48599 | 14 | 11380.47 | normal | S1AcK20dMeY88P         | 18 | 15 | 242.58  | S,1;K,7;Y,1;         | 0 |
| 1712 | 79.29 | 810.4  | 812.5371 | 812.5382 | -1.30778 | 14 | 11356.53 | normal | R3dMeK5AcK8AcK20Me     | 23 | 42 | 497.52  | R,5;K,2;K,3;K,7;     | 0 |
| 1712 | 79.29 | 810.4  | 811.5394 | 811.5371 | 2.85098  | 14 | 11342.51 | normal | R3MeK5AcK8AcK20Me      | 48 | 63 | 887.32  | R,2;K,1;K,2;K,32;    | 0 |
| 1713 | 79.34 | 757.97 | 758.308  | 758.3018 | 8.191196 | 15 | 11354.52 | A77→P  | K8AcK16AcK20Me         | 17 | 26 | 236.99  | K,3;K,2;K,3;         | 0 |

|      |       |         |          |          |          |    |          |        |                   |    |    |         |                   |   |
|------|-------|---------|----------|----------|----------|----|----------|--------|-------------------|----|----|---------|-------------------|---|
| 1713 | 79.34 | 757.97  | 754.5657 | 754.5667 | -1.3467  | 15 | 11298.49 | A77→P  | K8Ac              | 19 | 21 | 324.99  | K,3;              | 0 |
| 1714 | 79.38 | 757.97  | 754.5657 | 754.5667 | -1.3467  | 15 | 11298.49 | A77→P  | K16Ac             | 18 | 41 | 328.54  | K,8;              | 0 |
| 1719 | 79.6  | 709.22  | 708.3471 | 708.3452 | 2.637038 | 16 | 11312.52 | A77→P  | R3MeK12Ac         | 19 | 25 | 297.45  | R,2;K,2;          | 0 |
| 1719 | 79.6  | 709.22  | 710.1001 | 710.0972 | 4.08628  | 16 | 11340.55 | A77→P  | K12AcK20tMe       | 20 | 37 | 343.09  | K,3;K,2;          | 0 |
| 1719 | 79.6  | 709.22  | 710.1001 | 710.0972 | 4.08628  | 16 | 11340.55 | A77→P  | K5AcK20tMe        | 24 | 40 | 400.24  | K,2;K,10;         | 0 |
| 1719 | 79.6  | 709.22  | 710.1001 | 710.0972 | 4.08628  | 16 | 11340.55 | A77→P  | R3dMeK16AcK20Me   | 14 | 31 | 267.31  | R,2;K,6;K,6;      | 1 |
| 1722 | 79.73 | 874.42  | 871.5823 | 871.577  | 6.108916 | 13 | 11312.49 | A77→P  | K16AcK20Me        | 21 | 27 | 247.72  | K,2;K,2;          | 1 |
| 1722 | 79.73 | 874.42  | 873.8877 | 873.8883 | -0.6416  | 13 | 11342.54 | normal | R3dMeK5AcK20tMe   | 51 | 33 | 1011.29 | R,3;K,1;K,26;     | 0 |
| 1722 | 79.73 | 874.42  | 873.8877 | 873.8855 | 2.561334 | 13 | 11342.5  | normal | R3dMeK5AcK8Ac     | 53 | 40 | 1049.27 | R,3;K,1;K,1;      | 0 |
| 1724 | 79.83 | 754.7   | 756.2958 | 756.2971 | -1.71313 | 15 | 11324.45 | normal | K20MeY88P         | 12 | 17 | 239.61  | K,6;Y,2;          | 0 |
| 1725 | 79.87 | 754.7   | 757.5037 | 757.5018 | 2.575762 | 15 | 11342.52 | normal | S1AcK16AcK20dMe   | 71 | 76 | 1490.33 | S,2;K,35;K,38;    | 0 |
| 1727 | 79.97 | 808.4   | 811.5394 | 811.5371 | 2.926189 | 14 | 11342.51 | normal | K5AcK12AcK20dMe   | 60 | 67 | 1097.12 | K,3;K,1;K,30;     | 0 |
| 1737 | 80.41 | 869.57  | 872.5021 | 872.4954 | 7.628917 | 13 | 11324.43 | normal | K20MeS47P         | 29 | 27 | 439.19  | K,6;S,1;          | 0 |
| 1737 | 80.41 | 869.57  | 872.5021 | 872.4954 | 7.628917 | 13 | 11324.43 | normal | R3MeS47P          | 30 | 27 | 465.63  | R,3;S,1;          | 0 |
| 1738 | 80.46 | 869.57  | 873.8887 | 873.8855 | 3.748672 | 13 | 11342.5  | normal | K5AcK8AcK20dMe    | 61 | 69 | 1214.52 | K,4;K,2;K,37;     | 0 |
| 1741 | 80.59 | 707.47  | 710.0998 | 710.0949 | 6.858915 | 16 | 11340.51 | A77→P  | S1AcK16Ac         | 29 | 52 | 452.62  | S,2;K,10;         | 0 |
| 1741 | 80.59 | 707.47  | 710.2227 | 710.2209 | 2.55876  | 16 | 11342.53 | normal | S1AcR3MeK5AcK20Me | 61 | 83 | 1275.37 | S,0;R,2;K,2;K,38; | 1 |
| 1742 | 80.63 | 945.38  | 945.4698 | 945.4603 | 10.07724 | 12 | 11328.52 | normal | R3MeK12AcK20tMe   | 32 | 29 | 461.3   | R,3;K,2;K,1;      | 0 |
| 1742 | 80.63 | 945.38  | 941.9528 | 941.9564 | -3.80716 | 12 | 11286.47 | normal | K16AcK20Me        | 34 | 27 | 552.91  | K,6;K,6;          | 1 |
| 1742 | 80.63 | 945.38  | 941.9528 | 941.9564 | -3.80716 | 12 | 11286.47 | normal | R3MeK12Ac         | 36 | 23 | 568.78  | R,3;K,1;          | 0 |
| 1742 | 80.63 | 945.38  | 947.6256 | 947.6283 | -2.83091 | 12 | 11354.53 | A77→P  | R3MeK16AcK20tMe   | 19 | 22 | 267.56  | R,3;K,2;K,6;      | 2 |
| 1742 | 80.63 | 945.38  | 947.6256 | 947.6283 | -2.83091 | 12 | 11354.53 | A77→P  | R3MeK12AcK20tMe   | 19 | 22 | 246.3   | R,4;K,4;K,4;      | 0 |
| 1742 | 80.63 | 945.38  | 947.6256 | 947.6253 | 0.369715 | 12 | 11354.49 | A77→P  | R3MeK12AcK16Ac    | 19 | 20 | 241.61  | R,4;K,4;K,1;      | 0 |
| 1742 | 80.63 | 945.38  | 946.6268 | 946.6283 | -1.54437 | 12 | 11342.53 | normal | R3dMeK16AcK20tMe  | 52 | 26 | 1018.62 | R,0;K,24;K,25;    | 1 |
| 1744 | 80.73 | 1033.05 | 1031.139 | 1031.136 | 2.441981 | 11 | 11326.49 | A77→P  | R3dMeK12Ac        | 23 | 19 | 312.36  | R,2;K,2;          | 0 |
| 1751 | 81.05 | 872.73  | 871.5805 | 871.577  | 4.078092 | 13 | 11312.49 | A77→P  | R3MeK16Ac         | 25 | 16 | 278.59  | R,6;K,5;          | 0 |
| 1751 | 81.05 | 872.73  | 872.6578 | 872.6551 | 3.090429 | 13 | 11326.51 | A77→P  | R3MeK16AcK20Me    | 31 | 20 | 475.66  | R,6;K,11;K,10;    | 1 |

|      |       |        |          |          |          |    |          |        |                     |    |    |         |                   |   |
|------|-------|--------|----------|----------|----------|----|----------|--------|---------------------|----|----|---------|-------------------|---|
| 1751 | 81.05 | 872.73 | 873.7363 | 873.7332 | 3.573316 | 13 | 11340.52 | A77→P  | R3MeK16AcK20dMe     | 24 | 24 | 280.9   | R,6;K,4;K,3;      | 1 |
| 1751 | 81.05 | 872.73 | 873.8875 | 873.8855 | 2.351804 | 13 | 11342.5  | normal | R3MeK12AcK16AcK20Me | 54 | 35 | 1060.59 | R,4;K,0;K,0;K,24; | 2 |
| 1753 | 81.14 | 875.04 | 878.8096 | 878.8091 | 0.496482 | 13 | 11406.51 | A77→P  | S1PR3dMeK20tMe      | 21 | 12 | 256.55  | S,0;R,1;K,2;      | 1 |
| 1753 | 81.14 | 875.04 | 878.8096 | 878.8063 | 3.681485 | 13 | 11406.47 | A77→P  | K16AcK20dMeY88P     | 19 | 17 | 330.31  | K,11;K,11;Y,1;    | 0 |
| 1753 | 81.14 | 875.04 | 878.8096 | 878.8063 | 3.681485 | 13 | 11406.47 | A77→P  | K12AcK20dMeY88P     | 19 | 16 | 332.82  | K,1;K,11;Y,1;     | 0 |
| 1753 | 81.14 | 875.04 | 878.8096 | 878.8063 | 3.681485 | 13 | 11406.47 | A77→P  | S1AcK20dMeY88P      | 25 | 16 | 358     | S,1;K,11;Y,1;     | 0 |
| 1753 | 81.14 | 875.04 | 872.6578 | 872.6579 | -0.11702 | 13 | 11326.54 | A77→P  | R3dMeK20tMe         | 37 | 15 | 617.27  | R,4;K,2;          | 2 |
| 1753 | 81.14 | 875.04 | 872.6578 | 872.6551 | 3.090429 | 13 | 11326.51 | A77→P  | K16AcK20dMe         | 36 | 19 | 579.19  | K,13;K,14;        | 1 |
| 1753 | 81.14 | 875.04 | 872.6578 | 872.6551 | 3.090429 | 13 | 11326.51 | A77→P  | K12AcK20dMe         | 36 | 19 | 581.9   | K,1;K,14;         | 0 |
| 1753 | 81.14 | 875.04 | 872.6578 | 872.6551 | 3.090429 | 13 | 11326.51 | A77→P  | S1AcK20dMe          | 41 | 20 | 576.48  | S,1;K,14;         | 1 |
| 1754 | 81.18 | 875.04 | 877.8747 | 877.8833 | -9.75321 | 13 | 11394.47 | normal | S1PR3dMeK5AcK20Me   | 21 | 37 | 352.66  | S,0;R,0;K,0;K,3;  | 1 |
| 1754 | 81.18 | 875.04 | 878.9661 | 878.9614 | 5.393284 | 13 | 11408.49 | normal | S1PR3dMeK16AcK20dMe | 22 | 35 | 465.93  | S,0;R,1;K,2;K,5;  | 1 |
| 1754 | 81.18 | 875.04 | 874.9635 | 874.9636 | -0.09489 | 13 | 11356.52 | normal | K5AcK8AcK20tMe      | 31 | 38 | 608.22  | K,5;K,1;K,8;      | 0 |
| 1754 | 81.18 | 875.04 | 873.8875 | 873.8855 | 2.351804 | 13 | 11342.5  | normal | S1AcK8AcK20dMe      | 64 | 55 | 1218.46 | S,2;K,2;K,35;     | 0 |
| 1760 | 81.46 | 755.57 | 760.0211 | 760.0322 | -14.5215 | 15 | 11380.47 | normal | S1PK8AcK20dMe       | 20 | 44 | 322.09  | S,1;K,2;K,2;      | 0 |
| 1760 | 81.46 | 755.57 | 760.0211 | 760.0322 | -14.5215 | 15 | 11380.47 | normal | S1PR3MeK5AcK20Me    | 20 | 47 | 322.09  | S,1;R,2;K,2;K,2;  | 1 |
| 1760 | 81.46 | 755.57 | 760.0211 | 760.0322 | -14.5215 | 15 | 11380.47 | normal | S1PR3dMeK16Ac       | 18 | 42 | 281.98  | S,0;R,2;K,1;      | 1 |
| 1760 | 81.46 | 755.57 | 760.0211 | 760.0322 | -14.5215 | 15 | 11380.47 | normal | S1PR3dMeK5Ac        | 19 | 44 | 317.03  | S,0;R,2;K,2;      | 1 |
| 1760 | 81.46 | 755.57 | 757.504  | 757.5018 | 2.978634 | 15 | 11342.52 | normal | S1AcR3dMeK5Ac       | 53 | 61 | 1012.96 | S,0;R,2;K,2;      | 1 |
| 1767 | 81.78 | 711.1  | 710.2227 | 710.2209 | 2.55876  | 16 | 11342.53 | normal | S1AcK12AcK20dMe     | 69 | 74 | 1259.84 | S,2;K,1;K,39;     | 0 |
| 1770 | 81.92 | 947.8  | 945.1151 | 945.1194 | -4.58644 | 12 | 11324.42 | normal | S1PR3Me             | 34 | 31 | 500.55  | S,1;R,0;          | 3 |
| 1777 | 82.24 | 665.21 | 667.5624 | 667.5616 | 1.156342 | 17 | 11326.54 | A77→P  | R3dMeK16Ac          | 19 | 18 | 457.58  | R,2;K,13;         | 0 |
| 1778 | 82.28 | 665.21 | 669.21   | 669.2084 | 2.474525 | 17 | 11354.53 | A77→P  | S1AcK16AcK20Me      | 39 | 22 | 332.57  | S,2;K,11;K,5;     | 0 |
| 1784 | 82.56 | 810.9  | 809.3881 | 809.396  | -9.78315 | 14 | 11312.54 | A77→P  | R3MeK20tMe          | 23 | 23 | 315.78  | R,4;K,2;          | 1 |
| 1784 | 82.56 | 810.9  | 812.3928 | 812.3968 | -4.8926  | 14 | 11354.55 | A77→P  | R3dMeK8AcK20dMe     | 26 | 24 | 333.31  | R,5;K,1;K,7;      | 0 |
| 1784 | 82.56 | 810.9  | 810.3957 | 810.3946 | 1.395515 | 14 | 11326.52 | A77→P  | R3dMeK8Ac           | 28 | 37 | 496.22  | R,3;K,1;          | 0 |
| 1784 | 82.56 | 810.9  | 810.5387 | 810.5385 | 0.19899  | 14 | 11328.53 | normal | R3dMeK8AcK20dMe     | 35 | 41 | 588.86  | R,2;K,2;K,13;     | 0 |

|      |       |         |          |          |          |    |          |        |                     |    |    |        |                   |   |
|------|-------|---------|----------|----------|----------|----|----------|--------|---------------------|----|----|--------|-------------------|---|
| 1784 | 82.56 | 810.9   | 811.5378 | 811.5397 | -2.23304 | 14 | 11342.55 | normal | R3dMeK8AcK20tMe     | 51 | 43 | 994.67 | R,2;K,1;K,25;     | 0 |
| 1787 | 82.69 | 756.9   | 756.5695 | 756.5674 | 2.808795 | 15 | 11328.5  | normal | K5AcK12AcK20Me      | 33 | 58 | 571.94 | K,2;K,1;K,12;     | 0 |
| 1787 | 82.69 | 756.9   | 756.5695 | 756.5674 | 2.808795 | 15 | 11328.5  | normal | K5AcK8AcK20Me       | 31 | 57 | 571.94 | K,2;K,1;K,12;     | 0 |
| 1787 | 82.69 | 756.9   | 756.5695 | 756.5674 | 2.808795 | 15 | 11328.5  | normal | S1AcK8AcK20Me       | 34 | 56 | 610.52 | S,2;K,1;K,12;     | 0 |
| 1788 | 82.74 | 809.32  | 812.3928 | 812.3942 | -1.6922  | 14 | 11354.51 | A77→P  | K5AcK16AcK20Me      | 27 | 23 | 322.9  | K,4;K,6;K,6;      | 0 |
| 1788 | 82.74 | 809.32  | 810.3957 | 810.3946 | 1.395515 | 14 | 11326.52 | A77→P  | K5AcK20dMe          | 34 | 21 | 620.5  | K,4;K,13;         | 0 |
| 1788 | 82.74 | 809.32  | 810.3957 | 810.3946 | 1.395515 | 14 | 11326.52 | A77→P  | R3dMeK5Ac           | 30 | 21 | 562.33 | R,4;K,3;          | 0 |
| 1789 | 82.79 | 809.32  | 812.5334 | 812.5382 | -5.81478 | 14 | 11356.53 | normal | R3MeK5AcK12AcK20dMe | 27 | 40 | 649.31 | R,3;K,2;K,2;K,10; | 0 |
| 1789 | 82.79 | 809.32  | 810.5387 | 810.5385 | 0.19899  | 14 | 11328.53 | normal | R3dMeK12AcK20dMe    | 33 | 58 | 649.61 | R,2;K,1;K,12;     | 0 |
| 1789 | 82.79 | 809.32  | 810.5387 | 810.5359 | 3.406745 | 14 | 11328.49 | normal | K5AcK16AcK20Me      | 44 | 59 | 655.13 | K,5;K,13;K,11;    | 0 |
| 1790 | 82.83 | 669.5   | 667.563  | 667.5616 | 2.070642 | 17 | 11326.54 | A77→P  | K8AcK20dMe          | 19 | 18 | 424.79 | K,2;K,10;         | 0 |
| 1790 | 82.83 | 669.5   | 667.6802 | 667.6802 | 0.094082 | 17 | 11328.55 | normal | R3dMeK5AcK20dMe     | 28 | 33 | 644.74 | R,1;K,2;K,15;     | 0 |
| 1791 | 82.88 | 669.5   | 667.6802 | 667.678  | 3.300717 | 17 | 11328.52 | normal | S1AcK16AcK20Me      | 55 | 58 | 708.11 | S,2;K,15;K,10;    | 0 |
| 1791 | 82.88 | 669.5   | 667.6802 | 667.678  | 3.300717 | 17 | 11328.52 | normal | S1AcK12AcK20Me      | 54 | 59 | 725.36 | S,2;K,2;K,11;     | 0 |
| 1791 | 82.88 | 669.5   | 667.6802 | 667.678  | 3.300717 | 17 | 11328.52 | normal | S1AcK5AcK20Me       | 51 | 54 | 791.96 | S,2;K,0;K,14;     | 1 |
| 1795 | 83.07 | 873.89  | 877.8912 | 877.8805 | 12.20817 | 13 | 11394.44 | normal | S1PK5AcK8Ac         | 29 | 20 | 376.42 | S,4;K,0;K,0;      | 1 |
| 1795 | 83.07 | 873.89  | 871.5784 | 871.5798 | -1.51544 | 13 | 11312.53 | A77→P  | R3dMeK20dMe         | 24 | 21 | 346.34 | R,3;K,5;          | 2 |
| 1795 | 83.07 | 873.89  | 871.5784 | 871.577  | 1.697126 | 13 | 11312.49 | A77→P  | K12AcK20Me          | 25 | 23 | 348.88 | K,1;K,6;          | 0 |
| 1796 | 83.1  | 873.89  | 877.8912 | 877.8833 | 9.018644 | 13 | 11394.47 | normal | S1PR3dMeK16AcK20Me  | 22 | 34 | 354.3  | S,0;R,0;K,2;K,3;  | 2 |
| 1796 | 83.1  | 873.89  | 874.9615 | 874.9636 | -2.32712 | 13 | 11356.52 | normal | R3MeK5AcK8AcK20dMe  | 29 | 39 | 606.83 | R,3;K,3;K,2;K,7;  | 0 |
| 1799 | 83.24 | 1421.68 | 1424.191 | 1424.183 | 5.818901 | 8  | 11380.46 | normal | S1PR3dMeK20tMe      | 26 | 18 | 343.31 | S,1;R,1;K,2;      | 0 |
| 1804 | 83.48 | 812.97  | 813.238  | 813.2471 | -11.1699 | 14 | 11366.45 | normal | S1PK5AcK20Me        | 16 | 47 | 272.8  | S,2;K,1;K,3;      | 1 |
| 1806 | 83.57 | 946.54  | 943.9531 | 943.9514 | 1.747934 | 12 | 11310.41 | normal | S1P                 | 27 | 22 | 404.59 | S,0;              | 5 |
| 1808 | 83.65 | 668.56  | 667.6806 | 667.678  | 3.849202 | 17 | 11328.52 | normal | S1AcR3MeK5Ac        | 19 | 19 | 408.15 | S,0;R,0;K,0;      | 1 |
| 1810 | 83.75 | 1261.72 | 1260.048 | 1260.054 | -4.67152 | 9  | 11326.48 | A77→P  | R3MeK12AcK20Me      | 22 | 13 | 261.04 | R,5;K,3;K,8;      | 0 |
| 1829 | 84.61 | 811.61  | 809.5349 | 809.5374 | -3.09422 | 14 | 11314.52 | normal | R3MeK8AcK20dMe      | 32 | 42 | 581.57 | R,3;K,4;K,12;     | 0 |
| 1830 | 84.66 | 810.39  | 813.5348 | 813.5393 | -5.53257 | 14 | 11370.54 | normal | R3MeK5AcK8AcK20tMe  | 26 | 24 | 364.67 | R,3;K,1;K,2;K,3;  | 0 |

|      |       |        |          |          |          |    |          |        |                     |    |    |        |                  |   |
|------|-------|--------|----------|----------|----------|----|----------|--------|---------------------|----|----|--------|------------------|---|
| 1834 | 84.84 | 708.47 | 711.8516 | 711.8492 | 3.384846 | 16 | 11368.58 | A77→P  | S1AcR3dMeK20tMe     | 18 | 16 | 268.97 | S,0;R,1;K,1;     | 1 |
| 1835 | 84.89 | 708.47 | 711.9707 | 711.9706 | 0.170126 | 16 | 11370.52 | normal | K5AcK8AcK12AcK20Me  | 27 | 55 | 524.59 | K,2;K,2;K,1;K,6; | 0 |
| 1835 | 84.89 | 708.47 | 711.9707 | 711.9706 | 0.170126 | 16 | 11370.52 | normal | S1AcK8AcK12AcK20Me  | 28 | 53 | 489.42 | S,2;K,2;K,1;K,6; | 0 |
| 1835 | 84.89 | 708.47 | 708.4698 | 708.4712 | -1.93144 | 16 | 11314.53 | normal | R3dMeK12AcK20Me     | 31 | 63 | 588.14 | R,1;K,1;K,10;    | 0 |
| 1835 | 84.89 | 708.47 | 708.4698 | 708.4689 | 1.279707 | 16 | 11314.49 | normal | K5AcK8Ac            | 42 | 70 | 697.1  | K,2;K,2;         | 0 |
| 1835 | 84.89 | 708.47 | 710.0981 | 710.0949 | 4.452216 | 16 | 11340.51 | A77→P  | K5AcK8Ac            | 24 | 73 | 309.15 | K,2;K,2;         | 0 |
| 1840 | 85.11 | 757.5  | 752.8353 | 752.8323 | 3.923999 | 15 | 11272.48 | normal | K8Ac                | 20 | 53 | 302.38 | K,3;             | 0 |
| 1840 | 85.11 | 757.5  | 756.569  | 756.5698 | -1.0445  | 15 | 11328.54 | normal | R3MeK5AcK20tMe      | 25 | 48 | 521.63 | R,4;K,2;K,11;    | 0 |
| 1840 | 85.11 | 757.5  | 756.569  | 756.5674 | 2.163405 | 15 | 11328.5  | normal | R3MeK5AcK16Ac       | 28 | 51 | 581.6  | R,4;K,2;K,9;     | 0 |
| 1841 | 85.16 | 944.29 | 941.9515 | 941.9594 | -8.45254 | 12 | 11286.5  | normal | R3MeK20tMe          | 35 | 23 | 584.3  | R,1;K,3;         | 0 |
| 1841 | 85.16 | 944.29 | 945.4592 | 945.4603 | -1.15551 | 12 | 11328.52 | normal | R3MeK16AcK20tMe     | 34 | 19 | 556.89 | R,2;K,2;K,5;     | 1 |
| 1845 | 85.35 | 666.85 | 667.5616 | 667.5616 | -0.03225 | 17 | 11326.54 | A77→P  | S1AcR3MeK20Me       | 12 | 19 | 249.04 | S,0;R,1;K,6;     | 1 |
| 1845 | 85.35 | 666.85 | 666.7365 | 666.7372 | -1.0571  | 17 | 11312.52 | A77→P  | S1AcK20Me           | 18 | 23 | 370.76 | S,0;K,8;         | 1 |
| 1845 | 85.35 | 666.85 | 666.8549 | 666.8557 | -1.29653 | 17 | 11314.54 | normal | S1AcR3dMeK20Me      | 24 | 34 | 597.14 | S,0;R,1;K,14;    | 1 |
| 1845 | 85.35 | 666.85 | 668.3854 | 668.3861 | -1.01741 | 17 | 11340.55 | A77→P  | S1AcR3dMeK20Me      | 16 | 23 | 362.29 | S,0;R,1;K,9;     | 1 |
| 1850 | 85.58 | 809.89 | 814.5371 | 814.5378 | -0.86015 | 14 | 11384.52 | normal | R3dMeK8AcK12AcK16Ac | 30 | 21 | 429.7  | R,2;K,0;K,0;K,0; | 1 |
| 1850 | 85.58 | 809.89 | 807.5349 | 807.5352 | -0.40732 | 14 | 11286.48 | normal | K8AcK20Me           | 30 | 27 | 419.91 | K,4;K,5;         | 0 |
| 1851 | 85.62 | 809.89 | 812.5358 | 812.5356 | 0.238268 | 14 | 11356.49 | normal | S1AcK5AcK16Ac       | 29 | 44 | 661.12 | S,2;K,3;K,7;     | 0 |
| 1851 | 85.62 | 809.89 | 809.5366 | 809.5374 | -1.05856 | 14 | 11314.52 | normal | K5AcK20tMe          | 43 | 58 | 848.44 | K,3;K,23;        | 0 |
| 1851 | 85.62 | 809.89 | 809.5366 | 809.5374 | -1.05856 | 14 | 11314.52 | normal | S1AcR3MeK20dMe      | 38 | 54 | 792.03 | S,0;R,1;K,21;    | 1 |
| 1851 | 85.62 | 809.89 | 809.5366 | 809.5348 | 2.153161 | 14 | 11314.48 | normal | K5AcK16Ac           | 49 | 60 | 928.23 | K,4;K,23;        | 0 |
| 1851 | 85.62 | 809.89 | 809.5366 | 809.5348 | 2.153161 | 14 | 11314.48 | normal | K5AcK12Ac           | 47 | 62 | 879.67 | K,4;K,4;         | 0 |
| 1851 | 85.62 | 809.89 | 809.5366 | 809.5348 | 2.153161 | 14 | 11314.48 | normal | S1AcK12Ac           | 49 | 62 | 891.07 | S,2;K,4;         | 0 |
| 1851 | 85.62 | 809.89 | 811.538  | 811.5371 | 1.121165 | 14 | 11342.51 | normal | R3dMeK5AcK16Ac      | 35 | 48 | 716.38 | R,3;K,1;K,17;    | 0 |
| 1854 | 85.76 | 945.37 | 944.2902 | 944.2924 | -2.25336 | 12 | 11314.5  | normal | R3MeK16AcK20dMe     | 38 | 29 | 670.9  | R,1;K,10;K,12;   | 1 |
| 1862 | 86.12 | 755.63 | 758.4329 | 758.4361 | -4.3348  | 15 | 11356.53 | normal | K5AcK12AcK20tMe     | 34 | 43 | 656.27 | K,2;K,2;K,9;     | 0 |
| 1864 | 86.22 | 709.28 | 708.4708 | 708.4689 | 2.571969 | 16 | 11314.49 | normal | S1AcK16Ac           | 58 | 69 | 954.14 | S,2;K,24;        | 0 |

|      |       |        |          |          |          |    |          |        |                      |    |    |        |                  |   |
|------|-------|--------|----------|----------|----------|----|----------|--------|----------------------|----|----|--------|------------------|---|
| 1865 | 86.26 | 872.81 | 877.1244 | 877.1198 | 5.188172 | 13 | 11384.55 | normal | R3dMeK8AcK16AcK20tMe | 35 | 17 | 559.39 | R,2;K,1;K,9;K,9; | 0 |
| 1865 | 86.26 | 872.81 | 871.7308 | 871.732  | -1.40763 | 13 | 11314.51 | normal | R3dMeK8AcK20Me       | 40 | 23 | 809.84 | R,3;K,1;K,13;    | 0 |
| 1865 | 86.26 | 872.81 | 871.7308 | 871.7292 | 1.804374 | 13 | 11314.47 | normal | K12AcK16Ac           | 42 | 23 | 849.72 | K,1;K,15;        | 0 |
| 1865 | 86.26 | 872.81 | 871.7308 | 871.7292 | 1.804374 | 13 | 11314.47 | normal | S1AcK8Ac             | 43 | 20 | 849.72 | S,1;K,1;         | 0 |
| 1867 | 86.35 | 875.11 | 873.7327 | 873.7332 | -0.61802 | 13 | 11340.52 | A77→P  | K16AcK20tMe          | 27 | 29 | 351.92 | K,9;K,9;         | 1 |
| 1867 | 86.35 | 875.11 | 873.7327 | 873.7332 | -0.61802 | 13 | 11340.52 | A77→P  | S1AcK20tMe           | 32 | 30 | 416.33 | S,1;K,11;        | 0 |
| 1867 | 86.35 | 875.11 | 871.7308 | 871.732  | -1.40763 | 13 | 11314.51 | normal | K16AcK20tMe          | 45 | 31 | 891.4  | K,17;K,18;       | 1 |
| 1867 | 86.35 | 875.11 | 871.7308 | 871.732  | -1.40763 | 13 | 11314.51 | normal | K12AcK20tMe          | 45 | 32 | 894.29 | K,2;K,1;         | 0 |
| 1867 | 86.35 | 875.11 | 871.7308 | 871.732  | -1.40763 | 13 | 11314.51 | normal | S1AcK20tMe           | 46 | 35 | 865.48 | S,1;K,17;        | 0 |
| 1873 | 86.63 | 758.5  | 759.1075 | 759.0978 | 12.8652  | 15 | 11366.46 | normal | S1PR3MeK16Ac         | 18 | 47 | 347.11 | S,2;R,0;K,6;     | 1 |
| 1873 | 86.63 | 758.5  | 761.9122 | 761.9009 | 14.78068 | 15 | 11408.51 | normal | S1PR3MeK16AcK20tMe   | 17 | 38 | 329.13 | S,0;R,1;K,3;K,5; | 1 |
| 1873 | 86.63 | 758.5  | 756.5668 | 756.5674 | -0.74085 | 15 | 11328.5  | normal | R3MeK12AcK16Ac       | 24 | 46 | 496.17 | R,2;K,1;K,7;     | 0 |
| 1873 | 86.63 | 758.5  | 757.371  | 757.3674 | 4.803105 | 15 | 11340.5  | A77→P  | S1AcK8Ac             | 26 | 44 | 321.98 | S,2;K,1;         | 0 |
| 1873 | 86.63 | 758.5  | 757.503  | 757.5042 | -1.59376 | 15 | 11342.55 | normal | R3dMeK12AcK20tMe     | 41 | 61 | 845.94 | R,2;K,1;K,4;     | 0 |
| 1873 | 86.63 | 758.5  | 757.503  | 757.5018 | 1.608871 | 15 | 11342.52 | normal | R3dMeK12AcK16Ac      | 46 | 60 | 897.75 | R,3;K,1;K,24;    | 0 |
| 1876 | 86.77 | 711.16 | 713.3364 | 713.3454 | -12.5931 | 16 | 11392.52 | A77→P  | R3dMeK20dMeY88P      | 14 | 17 | 253.57 | R,2;K,8;Y,1;     | 0 |
| 1888 | 87.31 | 756.37 | 759.2291 | 759.2386 | -12.5271 | 15 | 11368.57 | A77→P  | R3dMeK16AcK20tMe     | 21 | 46 | 233.29 | R,1;K,13;K,12;   | 1 |
| 1894 | 87.59 | 809.32 | 809.3941 | 809.3934 | 0.817901 | 14 | 11312.5  | A77→P  | K5AcK20Me            | 25 | 25 | 362.83 | K,3;K,7;         | 0 |
| 1894 | 87.59 | 809.32 | 811.3954 | 811.3931 | 2.84294  | 14 | 11340.49 | A77→P  | K5AcK12Ac            | 29 | 32 | 394    | K,3;K,1;         | 0 |
| 1894 | 87.59 | 809.32 | 811.3954 | 811.3931 | 2.84294  | 14 | 11340.49 | A77→P  | S1AcK12Ac            | 29 | 32 | 362.65 | S,1;K,1;         | 0 |
| 1894 | 87.59 | 809.32 | 811.3954 | 811.3931 | 2.84294  | 14 | 11340.49 | A77→P  | S1AcK5Ac             | 27 | 30 | 352.28 | S,1;K,2;         | 1 |
| 1895 | 87.63 | 809.32 | 813.5275 | 813.5367 | -11.3396 | 14 | 11370.51 | normal | S1AcK5AcK16AcK20Me   | 39 | 32 | 616.09 | S,2;K,1;K,4;K,4; | 0 |
| 1895 | 87.63 | 809.32 | 812.5351 | 812.5382 | -3.78663 | 14 | 11356.53 | normal | S1AcK12AcK20tMe      | 42 | 42 | 641    | S,2;K,3;K,4;     | 0 |
| 1895 | 87.63 | 809.32 | 811.5377 | 811.5371 | 0.820328 | 14 | 11342.51 | normal | S1AcK5AcK20dMe       | 56 | 54 | 875.18 | S,2;K,1;K,14;    | 1 |
| 1905 | 88.1  | 873.81 | 874.9606 | 874.9636 | -3.44324 | 13 | 11356.52 | normal | R3dMeK5AcK16AcK20Me  | 32 | 12 | 447.15 | R,3;K,2;K,1;K,2; | 0 |
| 1905 | 88.1  | 873.81 | 872.8082 | 872.8073 | 0.959552 | 13 | 11328.49 | normal | K12AcK16AcK20Me      | 40 | 24 | 697.28 | K,0;K,11;K,11;   | 1 |
| 1905 | 88.1  | 873.81 | 873.8848 | 873.8855 | -0.72131 | 13 | 11342.5  | normal | R3dMeK5AcK12Ac       | 43 | 19 | 750.43 | R,3;K,2;K,1;     | 0 |

|      |       |         |          |          |          |    |          |        |                    |    |    |         |                   |    |
|------|-------|---------|----------|----------|----------|----|----------|--------|--------------------|----|----|---------|-------------------|----|
| 1905 | 88.1  | 873.81  | 871.7307 | 871.732  | -1.47764 | 13 | 11314.51 | normal | R3dMeK16AcK20Me    | 50 | 19 | 1033.17 | R,2;K,20;K,21;    | 1  |
| 1905 | 88.1  | 873.81  | 871.7307 | 871.732  | -1.47764 | 13 | 11314.51 | normal | R3dMeK5AcK20Me     | 49 | 18 | 989.22  | R,2;K,1;K,20;     | 0  |
| 1910 | 88.32 | 812.75  | 809.5357 | 809.5348 | 1.097626 | 14 | 11314.48 | normal | S1AcK5Ac           | 42 | 60 | 654.31  | S,2;K,4;          | 1  |
| 1941 | 89.73 | 707.6   | 707.5953 | 707.5952 | 0.053532 | 16 | 11300.39 | normal | R3MeK5AcK20Me      | 42 | 66 | 668.59  | R,4;K,2;K,21;     | 0  |
| 1941 | 89.73 | 707.6   | 707.5953 | 707.5952 | 0.053532 | 16 | 11300.39 | normal | R3MeK12AcK20Me     | 40 | 70 | 627.27  | R,4;K,1;K,20;     | 0  |
| 1951 | 90.19 | 1414.68 | 1418.941 | 1418.927 | 9.892763 | 8  | 11338.35 | normal | K20dMeS47P         | 29 | 13 | 334.43  | K,4;S,3;          | 0  |
| 1951 | 90.19 | 1414.68 | 1418.941 | 1418.927 | 9.892763 | 8  | 11338.35 | normal | R3MeK20MeS47P      | 27 | 14 | 281.56  | R,1;K,2;S,2;      | 0  |
| 1958 | 90.51 | 629.14  | 626.7491 | 626.7516 | -3.92259 | 18 | 11258.38 | normal | R3dMe              | 35 | 67 | 602.4   | R,1;              | 1  |
| 1958 | 90.51 | 629.14  | 629.0868 | 629.0855 | 2.014022 | 18 | 11300.39 | normal | R3dMeK16Ac         | 61 | 78 | 1085.14 | R,1;K,28;         | 0  |
| 1964 | 90.76 | 869.58  | 870.6555 | 870.6539 | 1.8889   | 13 | 11300.39 | normal | K16AcK20dMe        | 55 | 30 | 1106.71 | K,24;K,25;        | 1  |
| 1980 | 91.47 | 706.66  | 708.4677 | 708.4712 | -5.03285 | 16 | 11314.41 | normal | R3MeK12AcK20dMe    | 30 | 55 | 684.78  | R,1;K,1;K,9;      | 0  |
| 1980 | 91.47 | 706.66  | 707.5974 | 707.5952 | 2.986275 | 16 | 11300.39 | normal | K12AcK20dMe        | 67 | 82 | 1213.77 | K,5;K,30;         | 0  |
| 1983 | 91.6  | 805.32  | 809.5352 | 809.5374 | -2.71725 | 14 | 11314.41 | normal | R3MeK5AcK20dMe     | 34 | 40 | 783.93  | R,4;K,2;K,11;     | 0  |
| 1983 | 91.6  | 805.32  | 807.5383 | 807.5378 | 0.682418 | 14 | 11286.41 | normal | R3dMeK20dMe        | 38 | 30 | 761.64  | R,2;K,13;         | 10 |
| 1983 | 91.6  | 805.32  | 808.5394 | 808.5363 | 3.872072 | 14 | 11300.39 | normal | S1AcK20dMe         | 74 | 69 | 1483.43 | S,2;K,36;         | 3  |
| 1987 | 91.78 | 804.32  | 808.5394 | 808.5363 | 3.872072 | 14 | 11300.39 | normal | S1AcR3MeK20Me      | 49 | 53 | 946.13  | S,1;R,3;K,28;     | 1  |
| 1994 | 92.1  | 808.54  | 812.5302 | 812.5382 | -9.79597 | 14 | 11356.42 | normal | S1AcR3MeK5AcK20dMe | 23 | 47 | 538.27  | S,0;R,1;K,1;K,12; | 1  |
| 1995 | 92.14 | 807.47  | 808.538  | 808.5389 | -1.15533 | 14 | 11300.43 | normal | R3dMeK20tMe        | 55 | 32 | 1177.32 | R,1;K,1;          | 1  |
| 2010 | 92.83 | 941.79  | 939.6184 | 939.6235 | -5.41472 | 12 | 11258.38 | normal | K20dMe             | 42 | 32 | 776.2   | K,10;             | 7  |
| 2023 | 93.43 | 871.27  | 870.6548 | 870.6539 | 1.047668 | 13 | 11300.39 | normal | R3dMeK5Ac          | 60 | 23 | 1155.83 | R,3;K,1;          | 0  |
| 2023 | 93.43 | 871.27  | 867.4136 | 867.4223 | -9.97755 | 13 | 11258.38 | normal | R3MeK20Me          | 41 | 23 | 580.88  | R,3;K,8;          | 4  |
| 2060 | 95.1  | 870.65  | 871.7267 | 871.732  | -6.0987  | 13 | 11314.41 | normal | K8AcK20tMe         | 32 | 36 | 545.4   | K,6;K,8;          | 0  |
| 2060 | 95.1  | 870.65  | 870.6539 | 870.6539 | -0.00387 | 13 | 11300.39 | normal | R3dMeK12Ac         | 44 | 40 | 778.51  | R,2;K,1;          | 0  |
| 2064 | 95.29 | 943.13  | 944.2901 | 944.2893 | 0.829298 | 12 | 11314.37 | normal | K8AcK16Ac          | 26 | 34 | 436.28  | K,5;K,3;          | 0  |
| 2067 | 95.43 | 809.11  | 812.2457 | 812.2459 | -0.33918 | 14 | 11352.33 | normal | S1AcS47P           | 26 | 18 | 249.55  | S,1;S,1;          | 0  |
| 2100 | 96.93 | 942.29  | 938.468  | 938.4555 | 13.31185 | 12 | 11244.36 | normal | R3Me               | 36 | 22 | 557.7   | R,2;              | 2  |
| 2100 | 96.93 | 942.29  | 940.7839 | 940.7884 | -4.84752 | 12 | 11272.36 | normal | K16Ac              | 37 | 16 | 586.67  | K,6;              | 0  |

|      |        |        |          |          |          |    |          |        |                     |    |    |         |                  |      |
|------|--------|--------|----------|----------|----------|----|----------|--------|---------------------|----|----|---------|------------------|------|
| 2105 | 97.15  | 943.63 | 941.9555 | 941.9564 | -0.95613 | 12 | 11286.38 | normal | R3MeK16Ac           | 38 | 27 | 563.34  | R,3;K,5;         | 0    |
| 2111 | 97.43  | 755.17 | 759.0997 | 759.0978 | 2.573378 | 15 | 11366.34 | normal | S1AcK20MeY88P       | 20 | 16 | 271.17  | S,1;K,10;Y,1;    | 0    |
| 2120 | 97.84  | 871.88 | 868.3436 | 868.3454 | -2.00389 | 13 | 11270.38 | A77→P  | R3Me                | 24 | 19 | 296.67  | R,5;             | 3    |
| 2129 | 98.25  | 751.77 | 753.6349 | 753.6347 | 0.278292 | 15 | 11284.4  | A77→P  | R3MeK20Me           | 24 | 15 | 580.39  | R,2;K,14;        | 1    |
| 2130 | 98.3   | 751.77 | 754.7025 | 754.7011 | 1.9195   | 15 | 11300.39 | normal | K5AcK20dMe          | 62 | 63 | 1344.5  | K,2;K,33;        | 0    |
| 2136 | 98.58  | 754.64 | 754.7023 | 754.7011 | 1.596007 | 15 | 11300.39 | normal | R3dMeK8Ac           | 27 | 37 | 530.6   | R,4;K,2;         | 0    |
| 2138 | 98.66  | 809.68 | 807.3954 | 807.3938 | 2.034667 | 14 | 11284.4  | A77→P  | K20dMe              | 30 | 26 | 609.76  | K,14;            | 2    |
| 2138 | 98.66  | 809.68 | 807.3954 | 807.3938 | 2.034667 | 14 | 11284.4  | A77→P  | R3dMe               | 30 | 31 | 579.65  | R,3;             | 2    |
| 2138 | 98.66  | 809.68 | 807.5373 | 807.5352 | 2.615961 | 14 | 11286.38 | normal | K5AcK20Me           | 39 | 48 | 634.52  | K,2;K,12;        | 0    |
| 2144 | 98.94  | 941.71 | 937.2957 | 937.2876 | 8.708461 | 12 | 11230.35 | normal | null                | 33 | 28 | 480.22  | null             | null |
| 2144 | 98.94  | 941.71 | 938.4551 | 938.4555 | -0.47618 | 12 | 11244.36 | normal | K20Me               | 39 | 26 | 654.18  | K,8;             | 6    |
| 2144 | 98.94  | 941.71 | 946.2837 | 946.2874 | -3.87366 | 12 | 11338.35 | normal | S1PK20dMe           | 34 | 32 | 574.7   | S,0;K,6;         | 4    |
| 2167 | 99.99  | 704.09 | 706.7226 | 706.7193 | 4.719292 | 16 | 11286.38 | normal | K12AcK20Me          | 41 | 62 | 619.63  | K,6;K,8;         | 0    |
| 2167 | 99.99  | 704.09 | 706.7226 | 706.7193 | 4.719292 | 16 | 11286.38 | normal | S1AcK20Me           | 50 | 66 | 709.83  | S,2;K,9;         | 2    |
| 2180 | 100.58 | 870.65 | 872.646  | 872.6551 | -10.4084 | 13 | 11326.41 | A77→P  | R3MeK8AcK20Me       | 27 | 30 | 357.01  | R,3;K,1;K,12;    | 0    |
| 2180 | 100.58 | 870.65 | 870.655  | 870.6539 | 1.257976 | 13 | 11300.39 | normal | R3MeK16AcK20Me      | 51 | 35 | 1004.54 | R,3;K,25;K,27;   | 1    |
| 2180 | 100.58 | 870.65 | 870.655  | 870.6539 | 1.257976 | 13 | 11300.39 | normal | R3MeK8AcK20Me       | 50 | 36 | 995.79  | R,2;K,1;K,27;    | 0    |
| 2184 | 100.76 | 943.04 | 947.4562 | 947.4523 | 4.160413 | 12 | 11352.33 | normal | S1PK16Ac            | 26 | 20 | 368.56  | S,1;K,2;         | 0    |
| 2215 | 102.18 | 755.17 | 753.7684 | 753.7667 | 2.232232 | 15 | 11286.38 | normal | R3MeK8Ac            | 24 | 31 | 401.33  | R,3;K,1;         | 0    |
| 2225 | 102.64 | 808.61 | 812.5493 | 812.5382 | 13.71555 | 14 | 11356.42 | normal | S1AcR3MeK16AcK20dMe | 27 | 33 | 579.11  | S,1;R,4;K,5;K,6; | 0    |
| 2225 | 102.64 | 808.61 | 812.5493 | 812.5382 | 13.71555 | 14 | 11356.42 | normal | S1AcR3MeK12AcK20dMe | 27 | 36 | 570.97  | S,1;R,4;K,1;K,6; | 0    |
| 2225 | 102.64 | 808.61 | 810.5319 | 810.5385 | -8.15953 | 14 | 11328.42 | normal | S1AcR3MeK20tMe      | 21 | 34 | 393.77  | S,1;R,1;K,1;     | 0    |
| 2225 | 102.64 | 808.61 | 810.5319 | 810.5385 | -8.15953 | 14 | 11328.42 | normal | S1AcR3dMeK20dMe     | 26 | 36 | 557.69  | S,1;R,1;K,9;     | 1    |
| 2225 | 102.64 | 808.61 | 808.5385 | 808.5363 | 2.739745 | 14 | 11300.39 | normal | S1AcR3dMe           | 40 | 57 | 670.28  | S,1;R,2;         | 0    |
| 2231 | 102.92 | 807.61 | 811.5339 | 811.5397 | -7.04642 | 14 | 11342.44 | normal | S1AcR3dMeK20tMe     | 25 | 28 | 486.3   | S,1;R,4;K,4;     | 0    |
| 2238 | 103.24 | 751.97 | 756.5587 | 756.5698 | -14.6783 | 15 | 11328.42 | normal | R3MeK8AcK20tMe      | 22 | 40 | 409.81  | R,3;K,3;K,6;     | 0    |
| 2246 | 103.61 | 754.64 | 758.9716 | 758.9658 | 7.55056  | 15 | 11364.36 | A77→P  | S1PK20dMe           | 17 | 13 | 236.95  | S,3;K,2;         | 3    |

|      |        |         |          |          |          |    |          |           |                |    |    |         |              |      |
|------|--------|---------|----------|----------|----------|----|----------|-----------|----------------|----|----|---------|--------------|------|
| 2246 | 103.61 | 754.64  | 756.4332 | 756.4354 | -3.01083 | 15 | 11326.41 | A77→P     | S1AcR3dMe      | 24 | 26 | 398.5   | S,0;R,2;     | 1    |
| 2248 | 103.69 | 809.68  | 808.537  | 808.5363 | 0.928022 | 14 | 11300.39 | normal    | K8AcK20dMe     | 49 | 30 | 1048.63 | K,4;K,25;    | 0    |
| 2257 | 104.11 | 1416.06 | 1417.676 | 1417.682 | -4.22987 | 8  | 11328.39 | normal    | K8AcK16AcK20Me | 22 | 12 | 292.01  | K,2;K,2;K,3; | 0    |
| 2276 | 104.98 | 805.6   | 808.394  | 808.3923 | 2.052139 | 14 | 11298.38 | A77→P     | K5Ac           | 30 | 30 | 394.07  | K,3;         | 0    |
| 2290 | 105.63 | 870.65  | 868.3459 | 868.3454 | 0.667091 | 13 | 11270.38 | A77→P     | K20Me          | 22 | 20 | 322.81  | K,6;         | 1    |
| 2294 | 105.8  | 943.04  | 941.9536 | 941.9564 | -2.96481 | 12 | 11286.38 | normal    | S1AcR3Me       | 28 | 15 | 541.92  | S,0;R,0;     | 1    |
| 2340 | 107.91 | 871.88  | 870.5011 | 870.5016 | -0.60237 | 13 | 11298.41 | A77→P     | K20tMe         | 26 | 22 | 382.41  | K,11;        | 1    |
| 2340 | 107.91 | 871.88  | 870.5011 | 870.5016 | -0.60237 | 13 | 11298.41 | A77→P     | R3MeK20dMe     | 25 | 22 | 371.89  | R,2;K,10;    | 1    |
| 2340 | 107.91 | 871.88  | 870.5011 | 870.5016 | -0.60237 | 13 | 11298.41 | A77→P     | R3dMeK20Me     | 25 | 21 | 377.15  | R,2;K,10;    | 1    |
| 2340 | 107.91 | 871.88  | 870.5011 | 870.4988 | 2.614171 | 13 | 11298.38 | A77→P     | K12Ac          | 27 | 30 | 398.28  | K,1;         | 0    |
| 2340 | 107.91 | 871.88  | 870.5011 | 870.4988 | 2.614171 | 13 | 11298.38 | A77→P     | S1Ac           | 32 | 32 | 449.07  | S,1;         | 2    |
| 2342 | 108    | 807.53  | 806.5352 | 806.5367 | -1.79002 | 14 | 11272.4  | normal    | R3dMeK20Me     | 45 | 28 | 965.65  | R,2;K,21;    | 3    |
| 2342 | 108    | 807.53  | 806.5352 | 806.5341 | 1.433647 | 14 | 11272.36 | normal    | S1Ac           | 50 | 29 | 1037.29 | S,1;         | 2    |
| 2353 | 108.51 | 869.04  | 867.2643 | 867.2672 | -3.34008 | 13 | 11256.36 | A77→P     | null           | 21 | 20 | 328.64  | null         | null |
| 2353 | 108.51 | 869.04  | 868.4988 | 868.4976 | 1.40741  | 13 | 11272.36 | normal    | K12Ac          | 44 | 28 | 911.07  | K,1;         | 0    |
| 2358 | 108.73 | 809.68  | 806.5351 | 806.5341 | 1.282295 | 14 | 11272.36 | normal    | K5Ac           | 44 | 38 | 978.58  | K,3;         | 0    |
| 2384 | 109.93 | 807.03  | 806.5349 | 806.5367 | -2.1684  | 14 | 11272.4  | normal    | K20tMe         | 43 | 27 | 982.38  | K,22;        | 0    |
| 2384 | 109.93 | 807.03  | 806.5349 | 806.5367 | -2.1684  | 14 | 11272.4  | normal    | R3MeK20dMe     | 44 | 23 | 991.45  | R,1;K,22;    | 1    |
| 2479 | 114.31 | 811.46  | 814.1085 | 814.1042 | 5.302156 | 14 | 11378.34 | A77→P     | K5AcY88P       | 16 | 15 | 284.07  | K,2;Y,1;     | 0    |
| 2479 | 114.31 | 811.46  | 814.2472 | 814.2482 | -1.21169 | 14 | 11380.36 | normal    | R3dMeK5AcY88P  | 17 | 12 | 297.23  | R,3;K,1;Y,1; | 0    |
| 1543 | 71.6   | 814.47  | 818.6069 | 818.6052 | 2.043181 | 14 | 11441.46 | M+normal  | S2P            | 30 | 31 | 679.38  | S,0;         | 8    |
| 1579 | 73.24  | 948.96  | 948.2004 | 948.2076 | -7.52003 | 12 | 11361.48 | M+normal  | null           | 32 | 16 | 448.11  | null         | null |
| 1617 | 74.98  | 760.83  | 761.582  | 761.5708 | 14.81051 | 15 | 11404.56 | M+normal  | K21tMe         | 33 | 27 | 389.66  | K,0;         | 23   |
| 1568 | 72.74  | 813.61  | 814.7492 | 814.7516 | -2.91556 | 14 | 11387.51 | M+(A77→P) | null           | 19 | 26 | 201.82  | null         | null |
| 2462 | 113.52 | 702.15  | 702.5285 | 702.525  | 4.961272 | 16 | 11219.39 | R79→C     | S1Ac           | 24 | 16 | 195.79  | S,2;         | 2    |