

```

0      10      20      30      40      50      60
1  /* Peptide Fragment Size Calculation program */
2  /* To calculate the theoretical different peptide fragments */
3  /* by the given amino acid sequence and enzyme cleavage sites */
4  /* Program Composer: Alex Tzuu-Wang Chang */
5
6  #define Max_Protein_Sequence_Length 500
7  char BoNTA_LC[449] =
8  { 'M', 'P', 'F', 'V', 'N', 'K', 'Q', 'F', 'N', 'Y', 'K', 'D', 'P', 'V', 'N',
9    'G', 'V', 'D', 'I', 'A', 'Y', 'I', 'K', 'I', 'P', 'N', 'A', 'G', 'Q', 'M',
10   'Q', 'P', 'V', 'K', 'A', 'F', 'K', 'I', 'H', 'N', 'K', 'I', 'W', 'V', 'I',
11   'P', 'E', 'R', 'D', 'T', 'F', 'T', 'N', 'P', 'E', 'E', 'G', 'D', 'L', 'N',
12   'P', 'P', 'P', 'E', 'A', 'K', 'Q', 'V', 'P', 'V', 'S', 'Y', 'Y', 'D', 'S',
13   'T', 'Y', 'L', 'S', 'T', 'D', 'N', 'E', 'K', 'D', 'N', 'Y', 'L', 'K', 'G',
14   'V', 'T', 'K', 'L', 'F', 'E', 'R', 'I', 'Y', 'S', 'T', 'D', 'L', 'G', 'R',
15   'M', 'L', 'L', 'T', 'S', 'I', 'V', 'R', 'G', 'I', 'P', 'F', 'W', 'G', 'G',
16   'S', 'T', 'I', 'D', 'T', 'E', 'L', 'K', 'V', 'I', 'D', 'T', 'N', 'C', 'I',
17   'N', 'V', 'I', 'Q', 'P', 'D', 'G', 'S', 'Y', 'R', 'S', 'E', 'E', 'L', 'N',
18   'L', 'V', 'I', 'I', 'G', 'P', 'S', 'A', 'D', 'I', 'I', 'Q', 'F', 'E', 'C',
19   'K', 'S', 'F', 'G', 'H', 'E', 'V', 'L', 'N', 'L', 'T', 'R', 'N', 'G', 'Y',
20   'G', 'S', 'T', 'Q', 'Y', 'I', 'R', 'F', 'S', 'P', 'D', 'F', 'T', 'F', 'G',
21   'F', 'E', 'E', 'S', 'L', 'E', 'V', 'D', 'T', 'N', 'P', 'L', 'L', 'G', 'A',
22   'G', 'K', 'F', 'A', 'T', 'D', 'P', 'A', 'V', 'T', 'L', 'A', 'H', 'E', 'L',
23   'I', 'H', 'A', 'G', 'H', 'R', 'L', 'Y', 'G', 'I', 'A', 'I', 'N', 'P', 'N',
24   'R', 'V', 'F', 'K', 'V', 'N', 'T', 'N', 'A', 'Y', 'Y', 'E', 'M', 'S', 'G',
25   'L', 'E', 'V', 'S', 'F', 'E', 'E', 'L', 'R', 'T', 'F', 'G', 'G', 'H', 'D',
26   'A', 'K', 'F', 'I', 'D', 'S', 'L', 'Q', 'E', 'N', 'E', 'F', 'R', 'L', 'Y',
27   'Y', 'Y', 'N', 'K', 'F', 'K', 'D', 'I', 'A', 'S', 'T', 'L', 'N', 'K', 'A',
28   'K', 'S', 'I', 'V', 'G', 'T', 'T', 'A', 'S', 'L', 'Q', 'Y', 'M', 'K', 'N',
29   'V', 'F', 'K', 'E', 'K', 'Y', 'L', 'L', 'S', 'E', 'D', 'T', 'S', 'G', 'K',
30   'F', 'S', 'V', 'D', 'K', 'L', 'K', 'F', 'D', 'K', 'L', 'Y', 'K', 'M', 'L',
31   'T', 'E', 'I', 'Y', 'T', 'E', 'D', 'N', 'F', 'V', 'K', 'F', 'F', 'K', 'V',
32   'L', 'N', 'R', 'K', 'T', 'Y', 'L', 'N', 'F', 'D', 'K', 'A', 'V', 'F', 'K',
33   'I', 'N', 'I', 'V', 'P', 'K', 'V', 'N', 'Y', 'T', 'I', 'Y', 'D', 'G', 'F',
34   'N', 'L', 'R', 'N', 'T', 'N', 'L', 'A', 'A', 'N', 'F', 'N', 'G', 'Q', 'N',
35   'T', 'E', 'I', 'N', 'N', 'M', 'N', 'F', 'T', 'K', 'L', 'K', 'N', 'F', 'T',
36   'G', 'L', 'F', 'E', 'F', 'Y', 'K', 'L', 'L', 'C', 'V', 'R', 'G', 'I', 'I',
37   'T', 'S', 'K', 'T', 'K', 'S', 'L', 'D', 'K', 'G', 'Y', 'N', 'K', '\0' };
38  int Pepsin_Sites[106]=
39  { 0, 2, 7, 35, 51, 58, 77, 78, 87, 88, 93, 94, 102, 103, 106, 108, 116, 126, 127,
40    148, 149, 150, 151, 162, 163, 167, 173, 174, 175, 192, 193, 194, 195, 196,
41    199, 200, 206, 208, 212, 213, 220, 221, 224, 242, 255, 256, 259, 260, 262,
42    263, 265, 272, 273, 276, 277, 281, 282, 284, 289, 290, 296, 297, 309, 310,
43    317, 321, 323, 330, 331, 335, 336, 338, 340, 341, 344, 353, 354, 356, 357,
44    360, 367, 368, 369, 374, 389, 390, 391, 392, 396, 397, 400, 401, 412, 413,
45    415, 416, 418, 421, 422, 423, 424, 425, 427, 428, 441, 448 };
46  int Chymotrypsin_Sites[111]=
47  { 0, 3, 8, 10, 21, 30, 36, 39, 43, 51, 59, 72, 73, 77, 78, 87, 88, 94, 95, 99, 103,

```

```

0      10      20      30      40      50      60
48      106,107,108,117,118,127,144,149,151,163,168,170,173,175,180,
49      185,188,192,194,196,200,207,208,213,221,223,225,227,230,232,
50      233,243,250,251,253,256,260,263,266,273,277,282,284,285,286,
51      287,290,297,310,312,313,317,321,322,323,331,336,338,341,342,
52      344,345,349,354,357,358,361,366,367,369,374,384,387,390,392,
53      397,401,411,413,416,419,422,423,425,426,428,429,442,446,448};
54      int Trypsin_Sites[55]=
55      {0,6,11,23,34,37,41,48,66,84,89,93,97,105,113,128,145,166,177,
56      187,212,231,241,244,264,272,283,289,291,299,301,314,318,320,
57      330,335,337,340,343,356,359,363,364,371,375,381,393,415,417,
58      427,432,438,440,444,448};
59
60      main()
61      {
62          static char PeptideFragment[500];
63          int index,first,last,i,j,k,w,counter;
64          float MW;
65          char AA;
66
67          printf("BoNT/A Light Chain Sequence:\n");
68          for (index=0; index<449; index++)
69              { printf("%c", BoNTA_LC[index]);}
70          printf("\n");
71
72          printf("\n\n\n");
73          i=0; j=1; k=0; w=0; first=0; last=0;
74          printf("BoNT-A_LC Digested by Pepsin\n");
75          for (i=0; i<106; i++)
76          {
77              first=Pepsin_Sites[i];
78              for (j=i+1; j<106; j++)
79              {
80                  last=Pepsin_Sites[j];
81                  w=0;
82                  /* printf("first=%d, last=%d ", first, last); */
83                  printf("Pepsin: ");
84                  MW=0.0; counter=0;
85                  for (k=first; k<=last-1; k++)
86                  {
87                      PeptideFragment[w]=BoNTA_LC[k];
88                      counter++;
89                      AA=PeptideFragment[w];
90                      switch (AA)
91                      {
92                          case 'A':
93                              MW=MW+89.09;
94                              break;

```

```

0      10      20      30      40      50
147         MW=MW+181.19;
148         break;
149         case 'V':
150             MW=MW+117.15;
151             break;
152         default:
153             printf("Unknown Amino Acid\n");
154     }
155     printf("%c", PeptideFragment[w++]);
156 }
157 MW=(MW-((counter-1)*18))/1000;
158 printf(" <From %d To %d>", first+1, k);
159 printf(" MW=%4.3f KDa\n", MW);
160 /* printf("\n"); */
161 }
162 }
163 printf("\n\n\n");
164 i=0; j=1; k=0; w=0; first=0; last=0;
165 printf("BoNT-A_LC Digested by Chymotrypsin\n");
166 for (i=0; i<111; i++)
167 {
168     first=Chymotrypsin_Sites[i];
169     for (j=i+1; j<111; j++)
170     {
171         last=Chymotrypsin_Sites[j];
172         w=0;
173         /* printf("first=%d, last=%d ", first, last); */
174         printf("Chymotrypsin: ");
175         MW=0.0; counter=0;
176         for (k=first; k<=last-1; k++)
177         {
178             PeptideFragment[w]=BoNTA_LC[k];
179             counter++;
180             AA=PeptideFragment[w];
181             switch (AA)
182             {
183                 case 'A':
184                     MW=MW+89.09;
185                     break;
186                 case 'R':
187                     MW=MW+174.20;
188                     break;
189                 case 'D':
190                     MW=MW+133.10;
191                     break;
192                 case 'N':
193                     MW=MW+132.12;

```

