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%A function for converting the sequence to discrete vector for lysine
function [DataM]=Encode4PMeS_AAI_disorder_PSSM(Seqp)
width=11;
AAindex=[ -0.591 -1.302 -0.733 1.570 -0.146;
-1.343 0.465 -0.862 -1.020 -0.255;
1.050 0.302 -3.656 -0.259 -3.242;
1.357 -1.453 1.477 0.113 -0.837;
-1.006 -0.590 1.891 -0.397 0.412;
-0.384 1.652 1.330 1.045 2.064;
0.336 -0.417 -1.673 -1.474 -0.078;
-1.239 -0.547 2.131 0.393 0.816;
1.831 -0.561 0.533 -0.277 1.648;
-1.019 -0.987 -1.505 1.266 -0.912;
-0.663 -1.524 2.219 -1.005 1.212;
0.945 0.828 1.299 -0.169 0.933;
0.189 2.081 -1.628 0.421 -1.392;
0.931 -0.179 -3.005 -0.503 -1.853;
1.538 -0.055 1.502 0.440 2.897;
-0.228 1.399 -4.760 0.670 -2.647;
-0.032 0.326 2.213 0.908 1.313;
-1.337 -0.279 -0.544 1.242 -1.262;
-0.595 0.009 0.672 -2.128 -0.184
0.260 0.830 3.097 -0.838 1.512];
AAindexset=(AAindex-ones(20,1)*min(AAindex))./(ones(20,1)*max(AAindex)-ones(20,1)*min(AAindex));
OSet='ACDEFGHIKLMNPQRSTVWY';
LastVMar=[];
    %%%converting the sequence to disorder sequence
    [orderans,temLastVMar1]=getdisorder(Seqp,11);
    %%%Amino Acid Factors
    temLastVMar2=zeros(1,5*width);
    %%%Obtaining the AAindex of AA in the sequence
    temLastVMar3=zeros(1,20*width);
    db='E:/blast/swissprot/swissprot.fasta';
    pssm=getPSSM(Seqp,db);
    newpssm=pssm';
    for i=1:length(temsequence)
        Pointsite=find(OSet==temsequence(i));
        temLastVMar2=AAindexset(Pointsite,:);
        temLastVMar3=1+exp(-newpssm(i,:));
    end
DataM=[temLastVMar1,temLastVMar2,temLastVMar3];
return

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%inputfile: fasta 格式的文件
%使用灰色模型 GM(2,1)
function GreyPSSM=Grey_PSSM_2(inputFile)

[heads,seqs]=fastaread(inputFile);
pssm=blastpssm(inputFile,'E:/NCBI/blast-2.2.25+/db/swissprot');
if ~ischar(heads)
    len = length(heads);
    GreyPSSM = zeros(len,60);
    for i = 1 : len
        matrix = 1./(1+exp(pssm{i}(:,1:20)));
        v = AAVector(seqs{i});
        for j = 1 : 20
            p = GM21Param(matrix(:,j));
            GreyPSSM(i,-2+j*3:j*3) = [abs(p(1)) abs(p(2)) abs(p(3))]*v(j);
        end
    end
else
    GreyPSSM = zeros(1,60);
    matrix = 1./(1+exp(pssm(:,1:20)));
    v = AAVector(seqs);
    for j = 1 : 20
        p = GM21Param(matrix(:,j));
        GreyPSSM(-2+j*3:j*3) = [abs(p(1)) abs(p(2)) abs(p(3))]*v(j);
    end
end
end

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function [orderans,orderscores]=getdisorder(seq,width)
%函数作用：获得蛋白质序列中各氨基酸的 disorder 的得分
seqfile='E:/XXuan/PTM/VSL2DIR/VSL2/tmpseqf.txt';
fid=fopen(seqfile,'w');
fprintf(fid,'%s',seq);
fclose(fid);
%cmd=sprintf('cd E:/XXuan/PTM/VSL2DIR/VSL2');
%system(cmd);
cmd=sprintf('java -jar vsl2.jar -s:%s -w:%d >testseq.pred',seqfile,width);
[oderans,status]=system(cmd);
fid=fopen('E:/XXuan/PTM/VSL2DIR/VSL2/testseq.pred','r');
flag=0;
while flag==0
    line=fgetl(fid);

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    if strcmp(line,'NO.    RES.    PREDICTION    DISORDER')==1
        flag=1;
        line=fgetl(fid);
    end
end
orderans=[];
orderscores=[];
while ~feof(fid)
    flag2=1;
    line=fgetl(fid);
    row=sscanf(line,'%d %s %f \n',3);
    if strcmp(line,'=====')==1
        flag2=0;
    end
    if length(row)==3&flag2>0
        numth=size(orderans,2)+1;
        orderans(numth).No=row(1);
        orderans(numth).AA=char(row(2));
        orderans(numth).Score=row(3);
        orderscores=[orderscores;row(3)];
    end
end
end
fclose(fid);

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function [pssm]=getPSSM(seq,swiss)
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%函数作用：获得蛋白质序列 seq，相对 swiss 数据库进行 psi-blast 搜索，生成的 PSSM 矩阵

%seq: 蛋白质序列,

%swiss: SwissProt 数据库所在位置

%pssm:返回的 20*L 矩阵，其中 L 表示序列长度，20 对应 20 种氨基酸:A R N D C Q E G H I L
K M F P S T W Y V

%注意：要在本机调用本函数，本机必须安装有 NCBI Blast 程序包以及对应的 swiss 数据库文件

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seqFile='c:/tmpseq.txt';
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fid=fopen(seqFile,'w');
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    fprintf(fid,'%s\r\n%s','MyProtein',seq);
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fclose(fid);
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cmd=sprintf('blastpgp -j 3 -i %s -d %s -Q C:/pssm.txt',seqFile,swiss);
```

```
[result,status]=system(cmd);
```

```
fid=fopen('C:/pssm.txt','r');
for i=1:3
    line=fgetl(fid);
end
pssm=zeros(0,20);
while ~feof(fid)
    line=fgetl(fid);
    row=sscanf(line,'%d %s %d %d %d %d %d
```