

params.pl for iXLINK

```
sub LoadParams{
  my $params=$_[0];
```

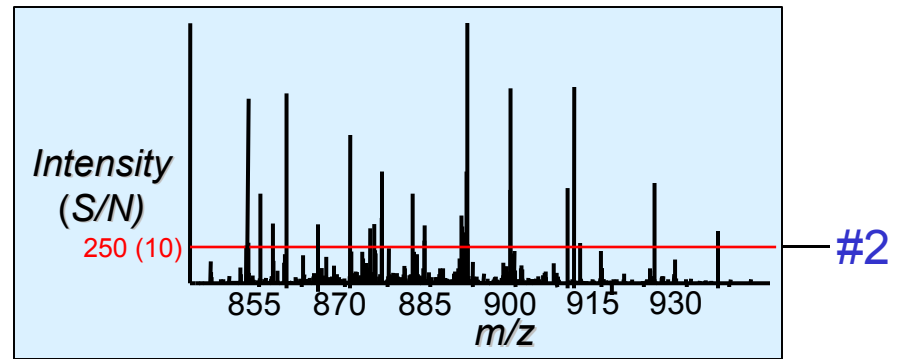
```
  $params->{aa_lib} = "aa_mass.txt";
  $params->{time_lib} = "timeConversion.txt";
```

```
  $params->{lonelyPeaksThreshold} = 500;
  $params->{lonelyPeaksSNRThreshold} = 200;
```

```
  $params->{signalThreshold} = 250;
  $params->{snrRatioThreshold} = 10;
  $params->{relativeIntensityRatio} = 5;
```

```
  $params->{pairDistance} = 12.02;
  $params->{pairDistanceError} = 0.2;
```

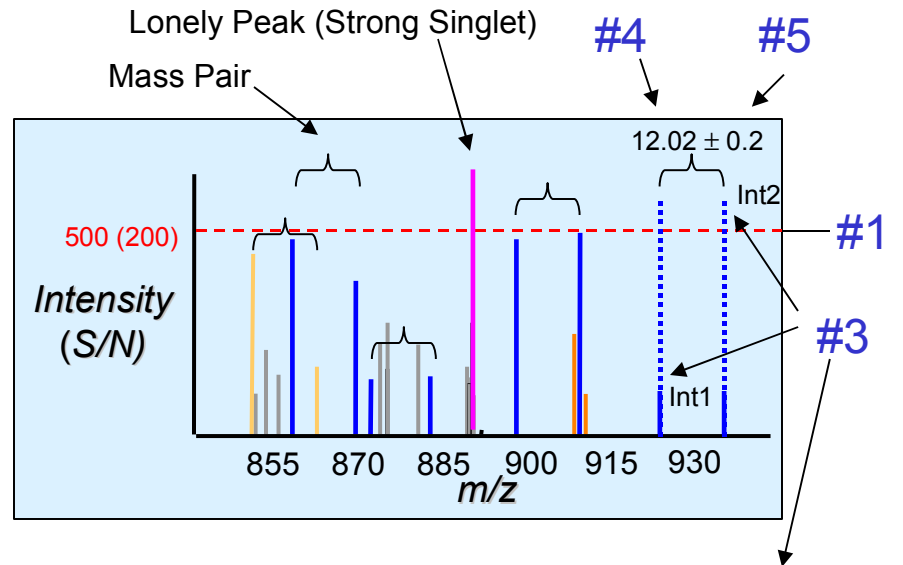
```
  ...
```



#1
#1

#2
#2
#3

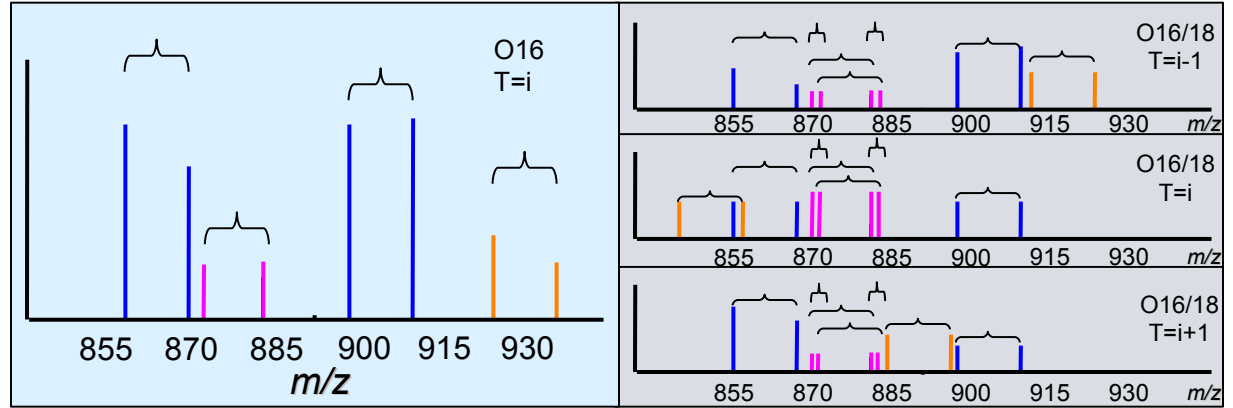
#4
#5



#3, relativeIntensityRatio = x: $1/x < \text{Int1} / \text{Int2} < x$

#: comments

#6 ← 2.0 ± 0.2 ← #7



[¹⁶O] spectrum of fraction at RT=i

[¹⁶O/¹⁸O] spectra of fractions around RT=i

#: comments

↔ : Constant Shift

⌈ : Range

...
 \$params->{heavyLightDistance} = 2.0; #6
 \$params->{heavyLightDistanceError} = 0.2; #7

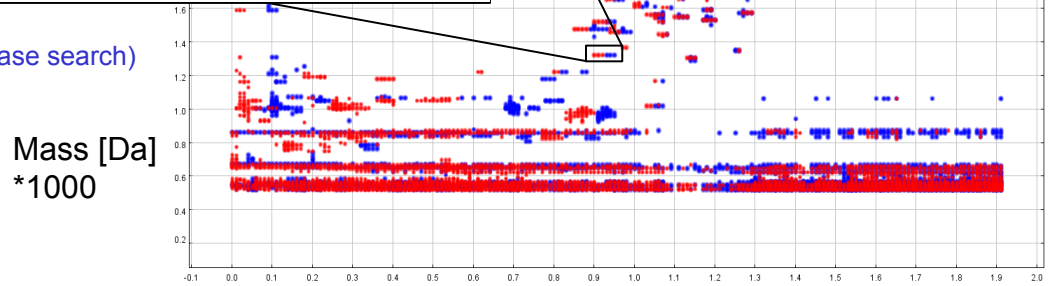
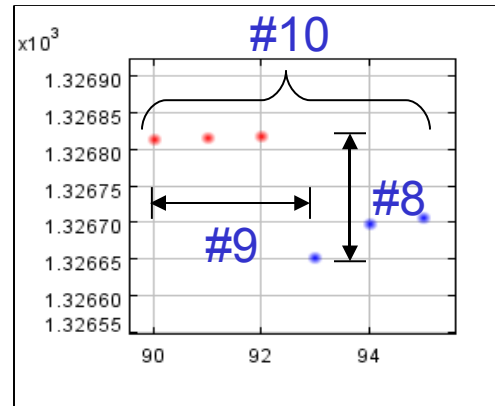
 \$params->{massCalibrationError} = 0.0; #8

 \$params->{heavyLightRTShift} = 0; #9
 \$params->{heavyLightRTErr} = 20; #10

 \$params->{IdentificationMassError} = 1.3; #11 (for Database search)

 \$params->{numberOfSpots} = 192; #12

 \$params->{SN_or_Inten} = "SN";
 ...



● [¹⁶O] LC-MS run

● [¹⁶O/¹⁸O] LC-MS run

Spot Position * 10

↑ #12

```
$params->{numberOfEnzymes} = 4; #12
```

```
$params->{enzymeName0} = "trypsin";  
$params->{enzymeSpecificity0} = "KR";  
$params->{enzymeSide0} = "c";
```

```
$params->{enzymeName1} = "aspn";  
$params->{enzymeSpecificity1} = "D";  
$params->{enzymeSide1} = "n";
```

```
$params->{enzymeName2} = "front";  
$params->{enzymeSpecificity2} = "n";  
$params->{enzymeSide2} = "n";
```

```
$params->{enzymeName3} = "back";  
$params->{enzymeSpecificity3} = "t";  
$params->{enzymeSide3} = "c";
```

```
$params->{numberOfReagents} = 1;
```

```
$params->{reagentName0} = "dss";  
$params->{reagentModifiesResidues0} = ("Kn");  
$params->{reagentMass0} = "156.0786";
```

```
# $params->{reagentName0} = "dsg";  
# $params->{reagentModifiesResidues0} = ("Kn");  
# $params->{reagentMass0} = "114.1";
```

```
$params->{minimumDigestMass} = "50";  
$params->{maximumDigestMass} = "4000";  
$params->{minimumXlinkMass} = "50";  
$params->{maximumXlinkMass} = "4000";
```

```
$params->{allowCysMods} = "1";  
$params->{allowMethMods} = "1";  
$params->{numAllowedMisCleavages} = 6;
```

```
...
```

Trypsin + Asp-N Digest

e.g. just Trypsin Digest

```
$params->{numberOfEnzymes} = 3;
```

```
$params->{enzymeName0} = "trypsin";  
$params->{enzymeSpecificity0} = "KR";  
$params->{enzymeSide0} = "c";
```

```
# $params->{enzymeName1} = "aspn";  
# $params->{enzymeSpecificity1} = "D";  
# $params->{enzymeSide1} = "n";
```

crosslinking reagent name
crosslinking reagent specificity, "n": N-terminus
mass added to peptide by crosslinking reagent (monolink)

crosslinking reagent name
crosslinking reagent specificity, "n": N-terminus
mass added to peptide by crosslinking reagent (monolink)

13: minimum mass calculated for peptides
13: maximum mass calculated for peptides
14: minimum mass calculated for crosslinked peptides
14: maximum mass calculated for crosslinked peptides

allow single cystein modification (e.g. carbomethylation, see also below ...), otherwise "0"
allow up to two methionine oxidations M# and M*, otherwise "0"
allow up to 6 missed cleavages per peptide

#: comments

```

if($params->{SN_or_Inten} eq "SN"){
    $params->{SN_or_Inten} = 2;
}
else{
    $params->{SN_or_Inten} = 1;
}
}

```

```

sub LoadMasses{

```

```

    my $massAtm = $_[0];

```

```

    ##avg

```

```

    #$massAtm->{'h'}= 1.00794; /* hydrogen */

```

```

    #$massAtm->{'o'}= 15.9994; /* oxygen */

```

```

    #$massAtm->{'c'}= 12.0107; /* carbon */

```

```

    #$massAtm->{'n'}= 14.00674; /* nitrogen */

```

```

    #$massAtm->{'p'}= 30.973761; /* phosphorus */

```

```

    #$massAtm->{'s'}= 32.066; /* sulphur */

```

```

    ##mono

```

```

    $massAtm->{'mass_h'}= 1.0078250;

```

```

    $massAtm->{'mass_o'}= 15.9949146;

```

```

    $massAtm->{'mass_c'}= 12.0000000;

```

```

    $massAtm->{'mass_n'}= 14.0030740;

```

```

    $massAtm->{'mass_p'}= 30.9737633;

```

```

    $massAtm->{'mass_s'}= 31.9720718;

```

```

    $massAtm->{'mass_nh3'} = $massAtm->{'mass_n'} + $massAtm->{'mass_h'} + $massAtm->{'mass_h'} + $massAtm->{'mass_h'};

```

```

    $massAtm->{'mass_co'} = $massAtm->{'mass_c'} + $massAtm->{'mass_o'};

```

```

    $massAtm->{'mass_co_2h'} = $massAtm->{'mass_co'} - $massAtm->{'mass_h'} - $massAtm->{'mass_h'};

```

```

    $massAtm->{'mass_Nterm'} = $massAtm->{'mass_h'};

```

```

    $massAtm->{'mass_Cterm'} = $massAtm->{'mass_o'} + $massAtm->{'mass_h'};

```

```

    $massAtm->{'mass_HOH'} = $massAtm->{'mass_o'} + $massAtm->{'mass_h'} + $massAtm->{'mass_h'};

```

```

    $massAtm->{'mass_HOOH'} = $massAtm->{'mass_o'} + $massAtm->{'mass_h'} + $massAtm->{'mass_h'} + $massAtm->{'mass_o'};

```

```

    $massAtm->{'mass_HH'} = $massAtm->{'mass_h'} + $massAtm->{'mass_h'}; ##check this!!!

```

```

    $massAtm->{'mass_termini'} = $massAtm->{'mass_Nterm'} + $massAtm->{'mass_Cterm'} + $massAtm->{'mass_h'}; /* peptide calc masses are MH+ */

```

```

    #$massAtm->{'TerminiMass'} = $dNterm + $dCterm ; /* peptide calc masses are M */

```

```

    $massAtm->{'cysMod'} = 57.02;

```

```

    $massAtm->{'metMod'} = $massAtm->{'mass_o'};

```

[#15: Cysteines alkylated with iod acetamide, carbamidomethylation](#)

1;

#: comments