

Define the isotopic contributions of each label

115a	115b	116a	116b
$x_{115a} := .9236$	$x_{115b} := .9392$	$x_{116a} := .9373$	$x_{116b} := .9429$
$y_{115a} := 0.0050$	$y_{115b} := 0.0033$	$y_{116a} := .0061$	$y_{116b} := .0085$
$z_{115a} := 0.0714$	$z_{115b} := 0.0575$	$z_{116a} := .0488$	$z_{116b} := .0485$
116c	117a	117b	117c
$x_{116c} := .8125$	$x_{117a} := .9403$	$x_{117b} := .8786$	$x_{117c} := .8907$
$y_{116c} := .1364$	$y_{117a} := .0079$	$y_{117b} := .0060$	$y_{117c} := .0028$
$z_{116c} := .0511$	$y_{117a} := .0074$	$y_{117b} := .0556$	$y_{117c} := .0547$
	$z_{117a} := .044$	$z_{117b} := .0598$	$z_{117c} := .0521$
118a	118b	118c	118d
$x_{118a} := .9412$	$x_{118b} := .8768$	$x_{118c} := .8990$	$x_{118d} := .9405$
$y_{118a} := .0066$	$y_{118b} := .0050$	$y_{118c} := .0092$	$y_{118d} := 0$
$z_{118a} := .0353$	$y_{118b} := .0057$	$y_{118c} := .0504$	$y_{118d} := .0041$
	$y_{118b} := .0637$	$z_{118c} := .0413$	$z_{118d} := .0554$
	$z_{118b} := .0487$		

x corresponds to reporter ion
y corresponds to -1 impurity
z corresponds to +1 impurity

Check these equations to verify that the isotopic contributions equal 1

$$\begin{aligned}
 x_{115a} + y_{115a} + z_{115a} &= 1 & x_{116c} + y_{116c} + z_{116c} &= 1 \\
 x_{115b} + y_{115b} + z_{115b} &= 1 & x_{117a} + y_{117a} + y_{117a} + z_{117a} &= \frac{2499}{2500} \\
 x_{116a} + y_{116a} + y_{116a} + z_{116a} &= 1 & x_{117b} + y_{117b} + y_{117b} + z_{117b} &= 1 \\
 x_{116b} + y_{116b} + z_{116b} &= \frac{9999}{10000} & x_{117c} + y_{117c} + y_{117c} + z_{117c} &= \frac{10003}{10000} \\
 x_{118a} + y_{118a} + y_{118a} + z_{118a} &= 1 & & \\
 x_{118b} + y_{118b} + y_{118b} + z_{118b} &= \frac{9999}{10000} & & \\
 x_{118c} + y_{118c} + y_{118c} + z_{118c} &= \frac{9999}{10000} & & \\
 x_{118d} + y_{118d} + y_{118d} + z_{118d} &= 1 & &
 \end{aligned}$$

The signal (S_{115a}) of each reporter ion is a combination of the following factors

Given

$$\begin{aligned}
 S_{115a} &= x_{115a} \cdot I_{115a} + y_{116a} \cdot I_{116a} \\
 S_{115b} &= x_{115b} \cdot I_{115b} + y_{116a} \cdot I_{116a} + y_{116b} \cdot I_{116b} \\
 S_{116a} &= x_{116a} \cdot I_{116a} + z_{115a} \cdot I_{115a} + y_{117a} \cdot I_{117a} \\
 S_{116b} &= x_{116b} \cdot I_{116b} + z_{115b} \cdot I_{115b} + y_{117a} \cdot I_{117a} \\
 S_{116c} &= x_{116c} \cdot I_{116c} + y_{117b} \cdot I_{117b} + y_{117c} \cdot I_{117c} \\
 S_{117a} &= x_{117a} \cdot I_{117a} + z_{116a} \cdot I_{116a} + y_{118a} \cdot I_{118a} \\
 S_{117b} &= x_{117b} \cdot I_{117b} + y_{118b} \cdot I_{118b} \\
 S_{117c} &= x_{117c} \cdot I_{117c} + z_{116c} \cdot I_{116c} + y_{118b} \cdot I_{118b} + y_{118c} \cdot I_{118c} \\
 S_{118a} &= x_{118a} \cdot I_{118a} + z_{117a} \cdot I_{117a} \\
 S_{118b} &= x_{118b} \cdot I_{118b} + z_{117b} \cdot I_{117b} \\
 S_{118c} &= x_{118c} \cdot I_{118c} + z_{117c} \cdot I_{117c} \\
 S_{118d} &= x_{118d} \cdot I_{118d}
 \end{aligned}$$

Find($I_{115a}, I_{115b}, I_{116a}, I_{116b}, I_{116c}, I_{117a}, I_{117b}, I_{117c}, I_{118a}, I_{118b}, I_{118c}, I_{118d}$) →

$$\left[\begin{aligned}
 &1.0834170670934283336 \cdot S_{115a} - 0.0090196522057480238117 \cdot S_{116a} + 0.000071042809813149932364 \cdot S_{117a} - 0.0000012756305629432998905 \cdot S_{118a} \\
 &0.00053686882856131098245 \cdot S_{115a} + 1.0653239013433464365 \cdot S_{115b} - 0.0069447065834625605517 \cdot S_{116a} - 0.0096036198551473589034 \cdot S_{116b} + 0.00013545298406283846168 \cdot S_{117a} - 0.0000024321668409073204446 \cdot S_{118a} \\
 &1.0680193304139583067 \cdot S_{116a} - 0.082564508652616525661 \cdot S_{115a} - 0.008412197326080163786 \cdot S_{117a} + 0.00015104774204287586909 \cdot S_{118a} \\
 &0.00088829501916367048432 \cdot S_{116a} - 0.064965663725996839641 \cdot S_{115b} - 0.00006867070633205508075 \cdot S_{115a} + 1.061143502112282292 \cdot S_{116b} - 0.0089297692873798687196 \cdot S_{117a} + 0.0001603411612374838306 \cdot S_{118a} \\
 &1.2310127575391317674 \cdot S_{116c} - 0.0084118679043524655708 \cdot S_{117b} - 0.003872123298328003963 \cdot S_{117c} + 0.000076765811526515822957 \cdot S_{118b} + 0.000039625733420041864805 \cdot S_{118c} \\
 &0.0042885634630657410314 \cdot S_{115a} - 0.055475031015231350373 \cdot S_{116a} + 1.0648216347451727853 \cdot S_{117a} - 0.01911972548575586493 \cdot S_{118a} \\
 &1.1386781998006741733 \cdot S_{117b} - 0.0074024472386677039097 \cdot S_{118b} \\
 &0.00091909767226187010186 \cdot S_{117b} - 0.070666250194486072325 \cdot S_{116c} + 1.1236072071041082928 \cdot S_{117c} - 0.0064134065833171009623 \cdot S_{118b} - 0.011498538715637148269 \cdot S_{118c} \\
 &0.002593392865140437119 \cdot S_{116a} - 0.00020048532976507926624 \cdot S_{115a} - 0.049779166945163198634 \cdot S_{117a} + 1.0633672629848844646 \cdot S_{118a} \\
 &1.1410158147181481851 \cdot S_{118b} - 0.077660762258303279614 \cdot S_{117b} \\
 &0.0040953410846860115329 \cdot S_{116c} - 0.000053264726056555542054 \cdot S_{117b} - 0.065116724683119067916 \cdot S_{117c} + 0.00037167795660825468313 \cdot S_{118b} + 1.1130134303304612852 \cdot S_{118c} \\
 &1.0632642211589580011 \cdot S_{118d}
 \end{aligned} \right]$$