

Modification Structure & Add Mass Calculation

Please complete and return the following form

User name: _____ Sample name: _____ Date: _____

In order for us to better understand and expedite your project, please provide the following information:

- *The structure, formula and monoisotopic molecular weight of the reagent*
- *The chemical reaction involved*
- *The **monoisotopic** molecular weight that is added to the protein, (“delta mass”, “net add weight”).*

Any additional information concerning the stability of the modified protein , e.g. acid, base, thermal or light lability, should be noted below. Please include the vendor and product number of the reagent, if possible. These steps insure that all lab members have a clear idea of both the structure and the chemistry involved. An example is provided on page 2.

REACTION OF REAGENT WITH PROTEIN (Please draw):

NET ADD MASS CALCULATION (List and calculate all masses as monoisotopic):

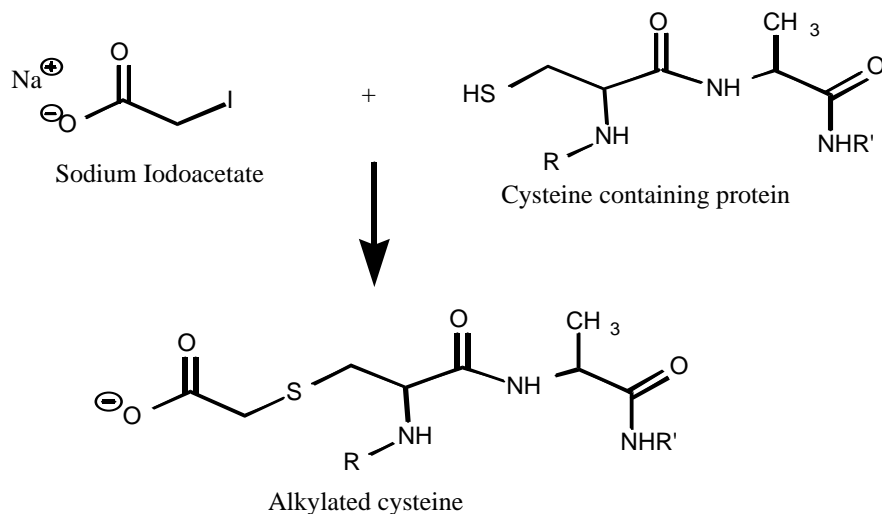
(A calculator can be found at <http://www.sisweb.com/cgi-bin/mass11.pl>. Choose high resolution)

Reagent source:	_____
Literature ref. (if needed)	_____
Molecular formula of reagent	_____
Molecular weight of neutral reagent	_____
MW of FULLY PROTONATED reagent	_____
Minus groups lost from reagent	_____
Plus groups gained by reagent	_____
Minus groups lost from protein	_____
Net add weight (monoisotopic & neutral)	_____

Please return this completed form to hmf@harvard.edu or fax 617-495-1374, and print a copy to accompany your sample when submitted.

Here is an example of how this form should be used to provide the information needed to determine a specific modified amino acid, in this example a derivatized cysteine.

REACTION OF REAGENT WITH PROTEIN



The modification is not acid, base or light sensitive.

List the following masses as Monoisotopic (<http://www.sisweb.com/cgi-bin/mass11.pl>) (Choose High Resolution)

Reagent source: Sigma I-6125

To calculate the add weight:

◆ Calculate the molecular weight of the FULLY PROTONATED REAGENT :	
e.g. sodium iodoacetate (C ₂ H ₂ O ₂ INa) =	207.9012
- sodium ion =	-22.9900
+ proton (C ₂ H ₃ O ₂ I) =	+1.0100
protonated reagent molecular weight =	<u>185.9212</u>
◆ Subtract the weight of any reagent groups lost during the reaction:	
e.g. -iodide ion =	-126.9000
net add weight =	<u>59.0200</u>
◆ Add the weight of any reagent groups gained during the reaction:	
e.g. no change in this case =	0.0000
◆ Subtract the weight of any protein groups lost during the reaction:	
e.g. -proton =	-1.0100
◆ The total is the add weight:	
e.g. Add weight =	<u>58.0100</u>