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 _____

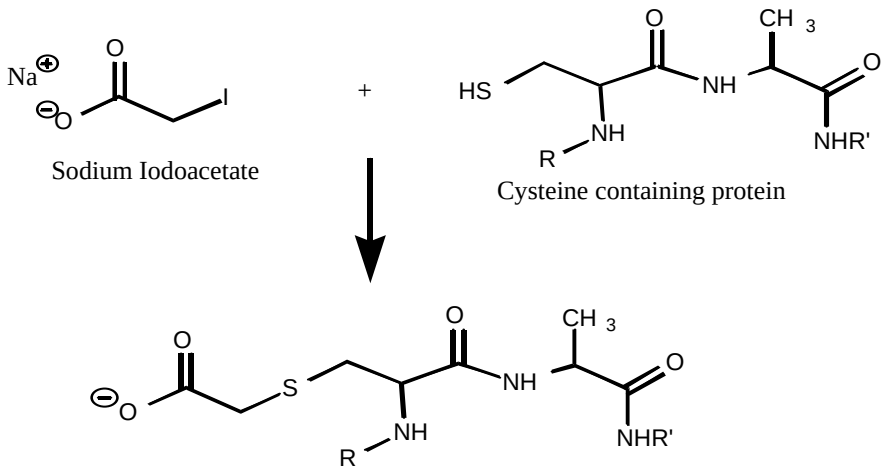
Minus groups lost from protein _____

Net add weight (monoisotopic & neutral) _____

Please return this completed form to proteomics@fas.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 ($C_2H_2O_2INa$) =	207.9012
	- sodium ion =	-22.9900
	+ proton ($C_2H_3O_2I$) =	+1.0100
	protonated reagent molecular weight =	185.9212

♦ Subtract the weight of any **reagent groups lost** during the reaction:

e.g.	-iodide ion =	-126.9000
	net add weight =	59.0200

♦ 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 =	**58.0100**