**Online Data for “A mass spectrometry approach for the identification and localization of small aldehyde modifications of proteins.”**

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The data files are divided into separate folders according to the protein and the aldehyde used and also the type of analysis (bottom-up approach or intact protein).

**LC-MSMS Data**

Folders:

* Bottom-up LC-MSMS HSA with acrolein
* Bottom-up LC-MSMS HSA with pentanal
* Bottom-up LC-MSMS Lysozyme with acrolein
* Bottom-up LC-MSMS Lysozyme with pentanal

Within these folders the files are named according to the aldehyde treatment concentration and time of reaction.

Example: R#\_Protein\_Aldehyde\_Time\_Concentration

For each treatment, there are 2 to 3 replicates (R1/R2/R3)

The data files were acquired on an ABSCIEX 5600 TripleTOF instrument and both wiff and wiff.scan files are supplied.

Bottom-up LC-MSMS HSA with acrolein

* R1\_HSA
* R1\_HSA\_Acrolein\_2h\_4mM
* R1\_HSA\_Acrolein\_2h\_8mM
* R1\_HSA\_Acrolein\_2h\_14mM
* R2\_HSA
* R2\_HSA\_Acrolein\_2h\_8mM
* R3\_HSA
* R3\_HSA\_Acrolein\_2h\_8mM

Bottom-up LC-MSMS HSA with pentanal

* R1\_HSA
* R1\_HSA\_Pentanal\_24h\_16\_6mM
* R2\_HSA
* R2\_HSA\_Pentanal\_24h\_16\_6mM

Bottom-up LC-MSMS Lysozyme with acrolein

* R1\_Lysozyme
* R1\_Lysozyme\_Acrolein\_2h\_4mM
* R1\_Lysozyme\_Acrolein\_2h\_8mM
* R1\_Lysozyme\_Acrolein\_2h\_14mM
* R2\_Lysozyme
* R2\_Lysozyme\_Acrolein\_2h\_4mM
* R2\_Lysozyme\_Acrolein\_2h\_8mM
* R2\_Lysozyme\_Acrolein\_2h\_14mM
* R3\_Lysozyme
* R3\_Lysozyme\_Acrolein\_2h\_4mM
* R3\_Lysozyme\_Acrolein\_2h\_8mM
* R3\_Lysozyme\_Acrolein\_2h\_14mM

Bottom-up LC-MSMS Lysozyme with pentanal

* R1\_Lysozyme
* R1\_Lysozyme\_Pentanal\_24h\_16.6M
* R2\_Lysozyme\_Pentanal\_24h\_16.6M
* R3\_Lysozyme\_Pentanal\_24h\_16.6M

**Intact Protein Data**

Folders:

* Intact Protein MS Lysozyme with acrolein
* Intact Protein MS Lysozyme with pentanal
* Supplementary Figure – DTT Reduction

Note: Some of the files contain multiple runs in a single file, some of them voided due to errors. The file name will present the protein and treatments of interest in each file. In this document the names of the runs of interest will follow the data file name:

Example:

* R#\_Protein\_Treatment\_(Time\_)Concentration(s)
  + Samples: Name of Sample(s) of interest within the file [if not obvious, translation of coded name]

Intact Protein MS Lysozyme reduction with DTT

* Lysozyme\_Native
  + Sample: lys
* R1\_Lysozyme\_DTT\_5mM\_10mM\_50mM\_100mM
  + Samples: 10mM, 100mM 2
* R2\_Lysozyme\_DTT\_10mM\_50mM\_100mM
  + Samples: sample 1 [10mM], Sample 3 [100mM]
* R3\_Lysozyme\_DTT\_Native\_1mM\_10mM\_50mM\_100mM
  + Samples: Lys 10mg/mL Zip tip2, Lys 10mM DTT ZipTip, Lys 50mM DTT ZipTip [mistake: is 100mM]
* R1\_Lysozyme\_DTT\_200mM
  + Sample: sample 2

Intact Protein MS Lysozyme with acrolein

* R1\_Lysozyme\_Acrolein\_2h\_4mM\_8mM\_14mM
  + Samples: Lys 4mM, Lys 8mM, Lys 14mM 2
* R2\_Lysozyme\_Acrolein\_2h\_4h\_8mM\_14mM
  + Samples: b 10ul 2h [8mM], b 20ul 2h [14mM]
* R3\_Lysozyme\_Acrolein\_2h\_8mM\_14mM
  + Samples: A [8mM], B [14mM]

Intact Protein MS Lysozyme with pentanal

* R1\_Lysozyme\_Pentanal\_24h\_16.6M
  + Samples: 1
* R2\_R3\_Lysozyme\_Pentanal\_24h\_16.6M
  + Samples: 24, 24’