

Validation of itaconate adducts on model proteins (Figure 5, Figures S8-S12)

To test the hypothesis that the +130 Da and +146 Da cysteine adducts discovered using SAMPEI in LPS stimulated macrophages were produced by itaconate, we reacted *in vitro* two model proteins (BSA and KEAP1) with the 0, 5mM, and 50mM of the metabolite. To improve sequence coverage the reacted proteins were digested in parallel with trypsin, GluC and elastase. Peptides were analyzed by high-resolution tandem mass spectrometry, and the spectra obtained were analyzed to confirm dose dependent formation of the +130 and +146 Da adducts.

Raw MS data are publicly available via the PRIDE repository with dataset identifiers PXD019858.

Files

The dataset contains SAMPEI identifications from each of the experimental conditions applied. Itaconate amount and protease used are specified in the file names.

The dataset contains the following files:

- 5mM_itaconate_elastase_V4.txt
- 50mM_itaconate_elastase_V4.txt
- neg_control_elastase_V4.txt
- 5mM_itaconate_trypsin_V4.txt
- 50mM_itaconate_trypsin_V4.txt
- neg_control_trypsin_V4.txt
- 5mM_itaconate_GluC_V4.txt
- 50mM_itaconate_GluC_V4.txt
- neg_control_GluC_V4.txt