

Large-Scale Quantitative Cross-Linking and Mass Spectrometry Provides New Insight on Protein Conformational Plasticity within Organelles, Cells, and Tissues

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SUPPORTING INFORMATION:

The following supporting information is available free of charge at ACS website

- Figure S1 – Cumulative distribution of DE peptide attached lysine residue DSSP accessibilities in structures.
- Figure S2 – Comparison of intra-protein quantitation clusters of ADT2_HUMAN and those of isoform ADT3_HUMAN and homologue ADT2_MOUSE.
- Figure S3 – ACADV1_MOUSE quantitation log₂ratios of cross-links spanning residues 277_483 and 279_483 with respect to 27 common compared samples in which they were confidently quantified.
- Video S1 – Training tutorial on how to view intra-protein quantitation clusters for *M. musculus* and *H. sapiens* proteins on XLinkDB.

Supporting Figures:

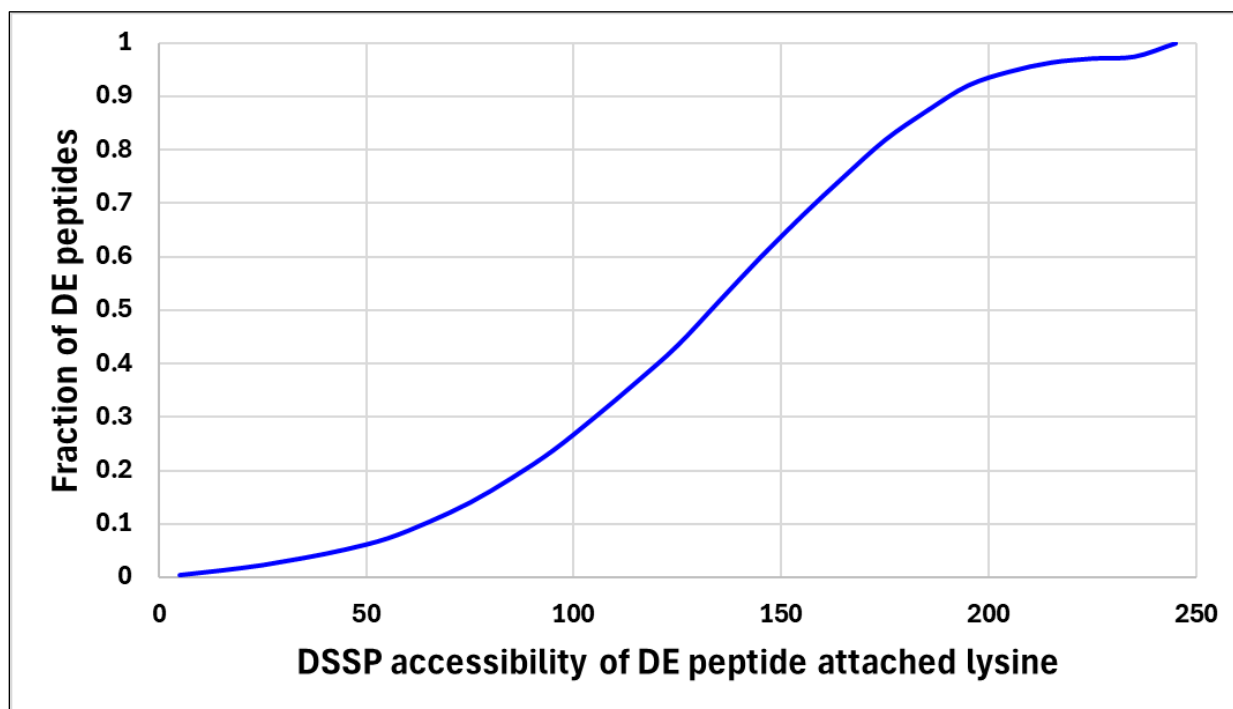


Figure S1. Cumulative distribution of DE peptide attached lysine residue DSSP accessibilities in structures. Shown is the fraction of 9,899 non-redundant DE peptides on XLinkDB with accessibilities in structures less than the indicated value on the x-axis. 95% of DE peptides have an accessibility in a structure of 50 or greater.

ADT2_HUMAN	ADT3_HUMAN	ADT2_MOUSE
23_33	23_33	23_33
23_272	23_272	23_272
33_147	33_147	33_147
33_245	33_245	
33_272	33_272	33_272
43_272	43_272	43_272
63_163	63_163	
147_272	147_272	147_272
163_272	163_272	
272_DE	272_DE	272_DE
23_92	23_92	23_92
23_94	23_94	23_94
23_96	23_96	23_96
23_105		23_105
23_DE	23_DE	23_DE
92_DE	92_DE	92_DE
92_96		92_96
92_105	92_105	92_105

Color Legend

ADT2_HUMAN Cluster 1: m-state
ADT2_HUMAN Cluster 2: c-state
ADT2_HUMAN Cluster 3: either state
ADT3_HUMAN Additional cluster
ADT2_MOUSE Additional cluster

Figure S2. Comparison of intra-protein quantitation clusters of ADT2_HUMAN and those of isoform ADT3_HUMAN and homologue ADT2_MOUSE. Shown are cross-links of ADT2_HUMAN (indicated by residue pair with _DE specifying a DE peptide) that were also assigned to clusters of ADT3_HUMAN and/or ADT2_MOUSE. Assigned clusters for cross-links of the three proteins are indicated by color as equivalent ADT2_HUMAN m-state specific (yellow), c-state specific (green), and state-insensitive (blue), as well as additional clusters of ADT3_HUMAN (pink) and ADT2_MOUSE (red) .

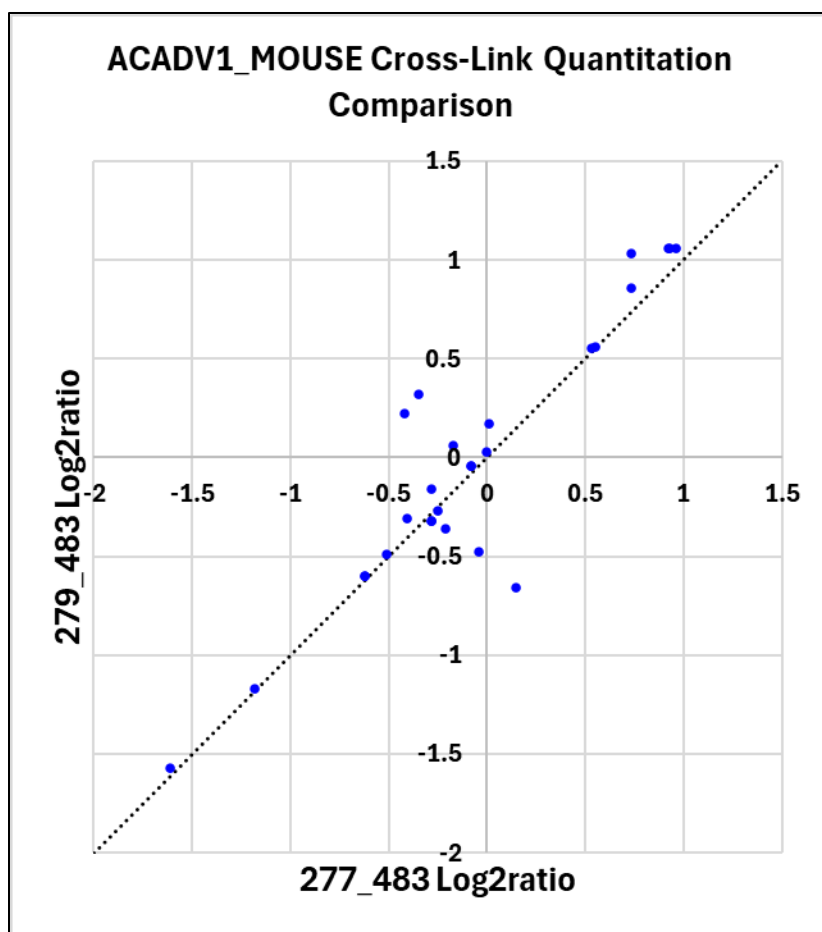


Figure S3. Comparison of quantitation log₂ratios of ACADV1_MOUSE cross-links spanning residues 277_483 and 279_483 with respect to 27 common compared samples in which they were both confidently quantified. The linear correlation R^2 is 0.84. The dashed line indicates equal log₂ratios.