

Observed Mass MH+ (Da): 1331.64429 Da, Observed Monoisotopic m/z: 666.32578 Da Peptide2 Sequence: LLVCAGEDGPLR, C4-SH->S-S-IAA (88.99300 Da), polysulfide-treated

Calculated Mass MH+ (Da): 1331.64413 Da, Calculated Monoisotopic m/z: 666.32572 Da

Identified with: Sequest HT (v1.17); XCorr:2.46, RT: 53.8333 min

Calculated Mass M (Da): 1330.63685 Da

**Figure S2.** MS<sup>2</sup> data of peptide 2 (Cys<sup>62</sup>-SH) (from HS<sub>n</sub>H treated AdpA).