Supporting Information

Reversibility of Covalent Electrophile-Protein Adducts and Chemical Toxicity

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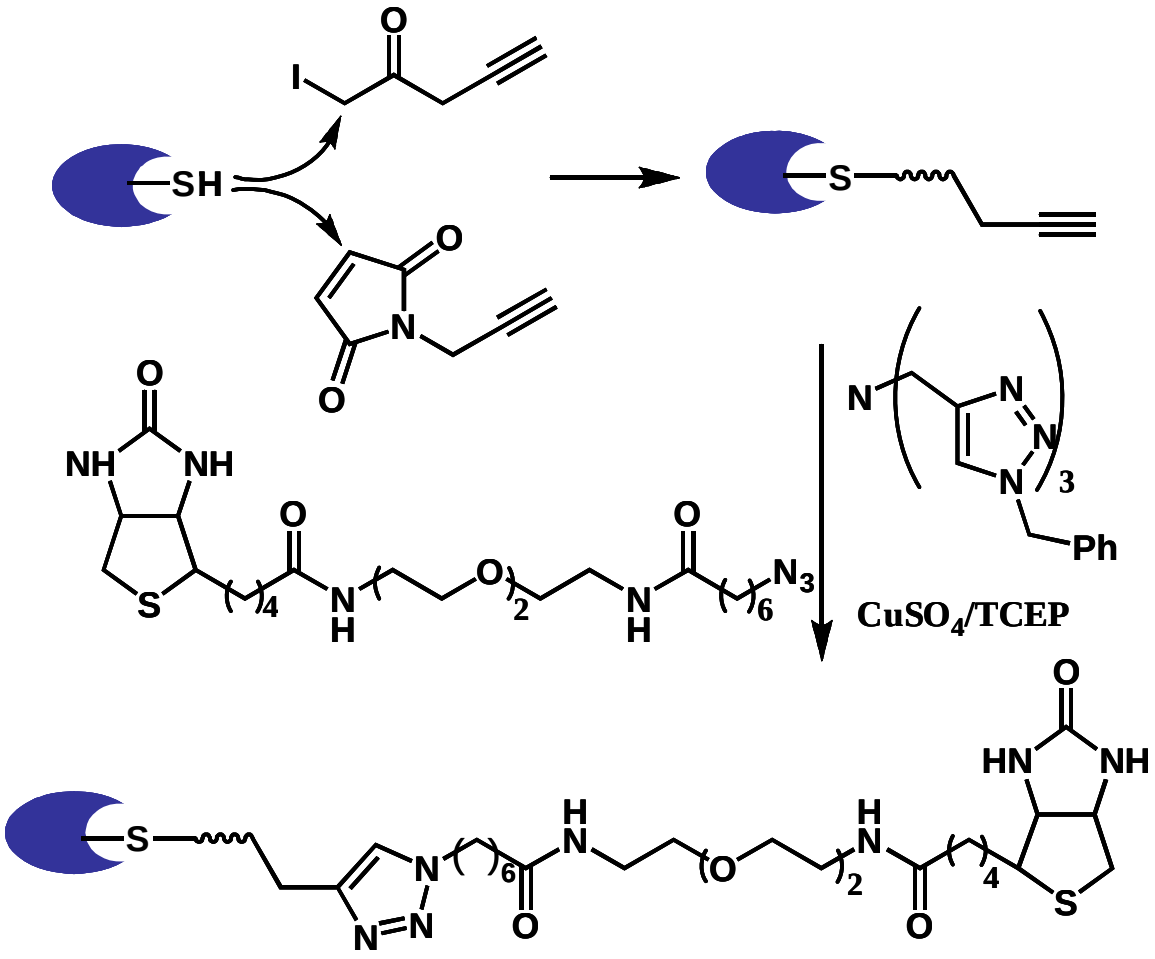
Scheme S1

Figures S1-S8

Scheme S1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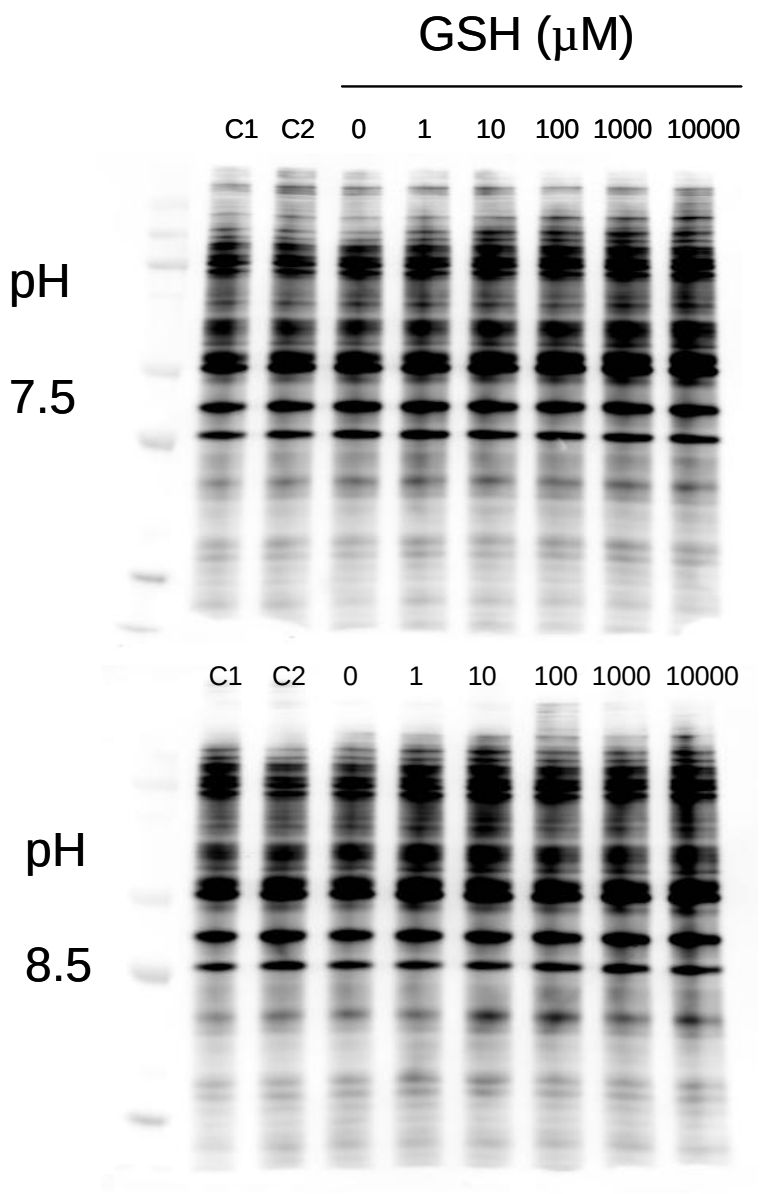

Figure S1. Stability of BMCC adducts from BMCC-pretreated HEK293 cell lysate (lysate treated with 10 μM BMCC for 1 h at 37 ^{o}C). The adduct-containing lysate protein was left either untreated (lane) or incubated with the indicated concentrations (μM) of GSH for 1 h at pH 7.5 (upper panel) and 8.5 (lower panel) at 37 °C. Lane labeled C2 represent 2 h pretreatment of lysate with BMCC at 37 ^{o}C.

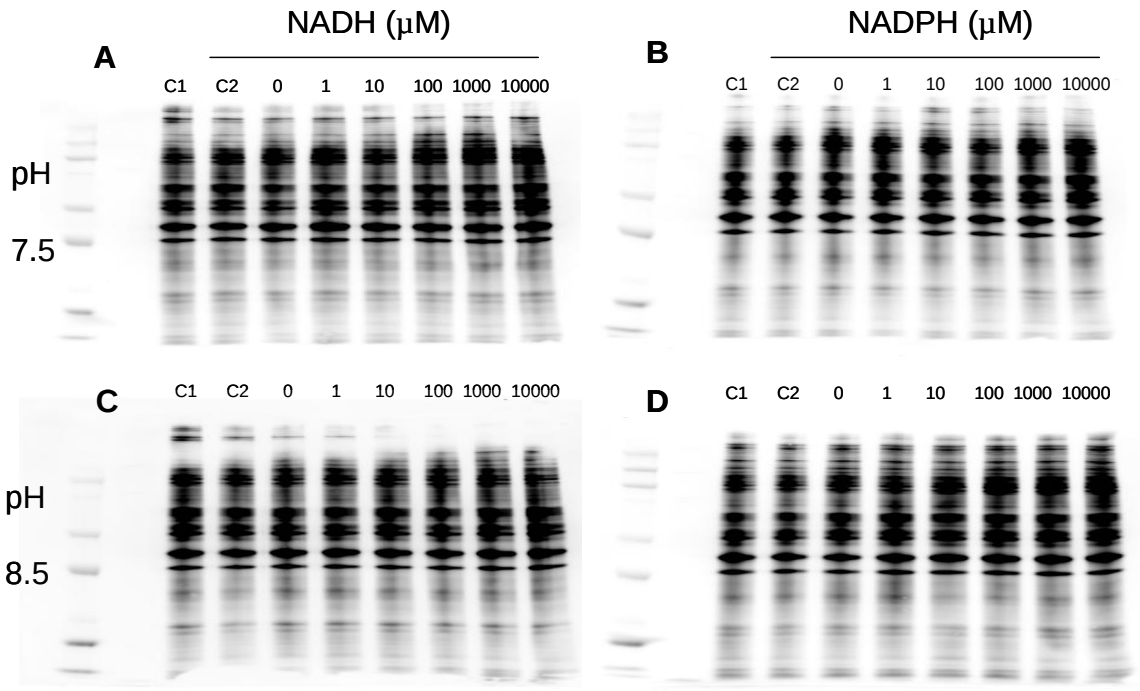

Figure S2. Stability of BMCC adducts from BMCC-pretreated HEK293 cell lysate (lysate treated with 10 μM BMCC for 1 h). The adduct-containing lysate protein was left either untreated (lane) or incubated with the indicated concentrations (μM) of NADH at pH 7.5 (A), 8.5 (C), NADPH at pH 7.5 (B), 8.5 (D) for 1 h at pH 7.5. Lanes labeled C2 represent 2 h pretreatment of lysate with BMCC at 37 ^{o}C.

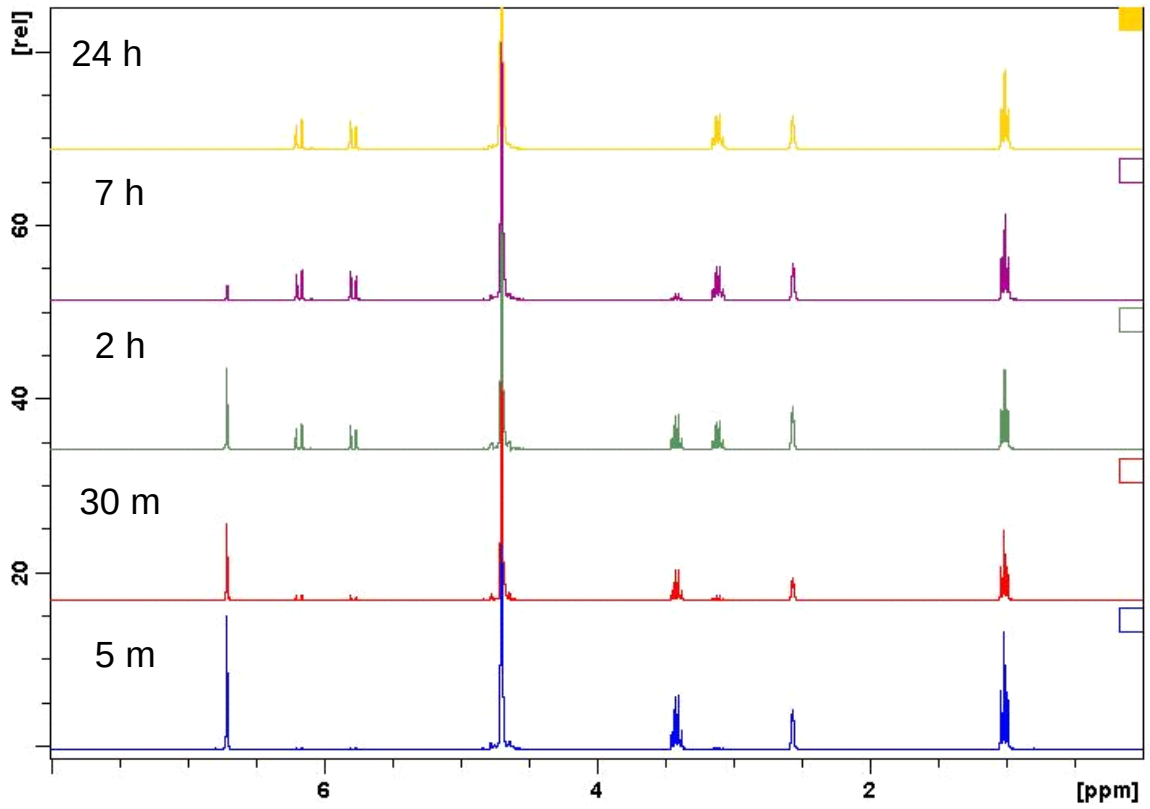

Figure S3. ^{1}H-NMR spectra for the conversion of NEM (10 mM) to its hydrolyzed acid form in 100 mM, pH 8.0 D_2O phosphate buffer containing 10% d_6-DMSO at 37 ^{o}C.

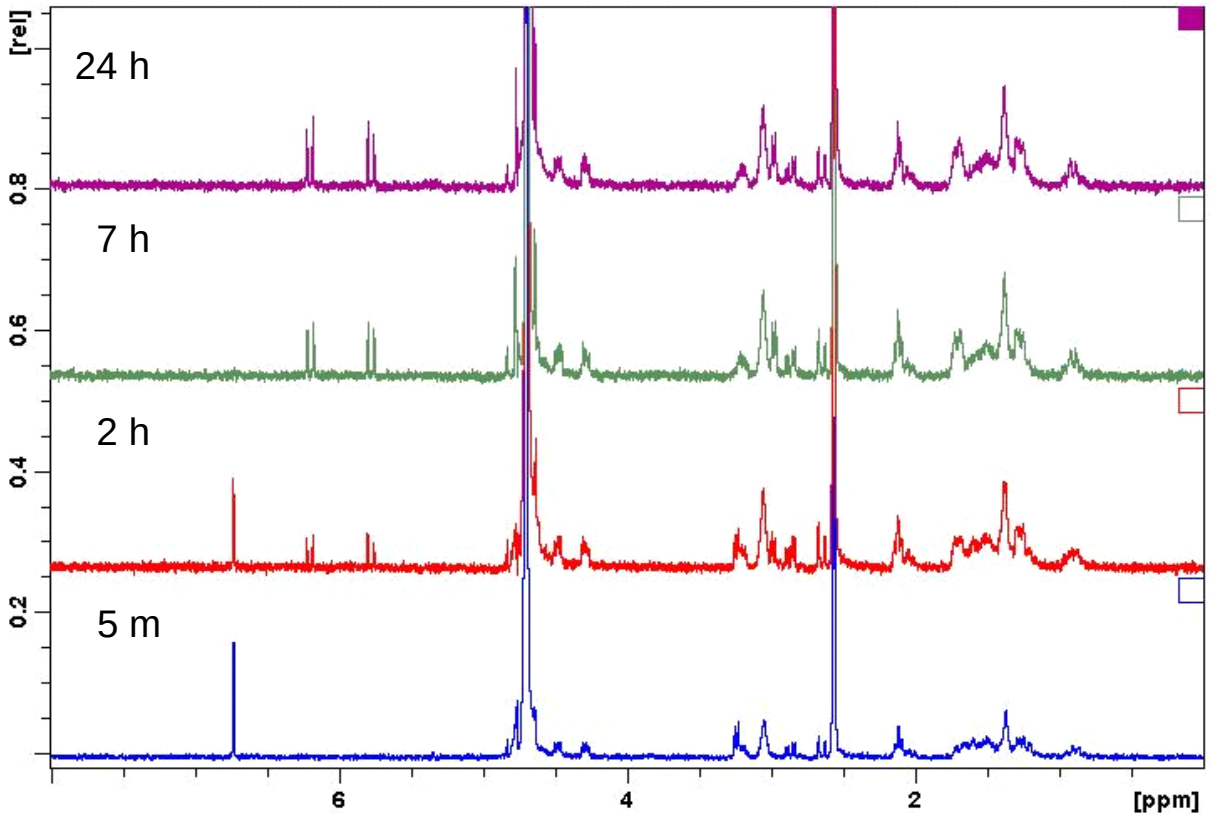

Figure S4. ^{1}H-NMR spectra for the conversion of BMCC (1 mM) to its acid form (BMCC-acid) in 100 mM, pH 8.0 D_2O-phosphate buffer containing 10% d_6-DMSO at 37 ^{o}C.

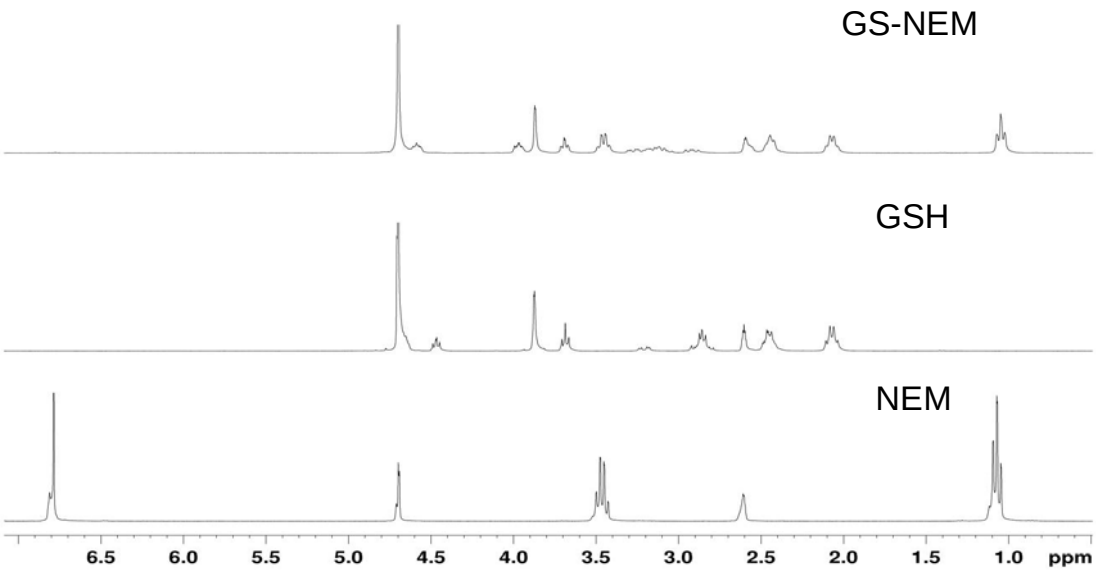

Figure S5. ^{1}H-NMR spectra for the conversion of NEM (40 mM) to its GSH conjugate GS-NEM in D_2O containing 28% d_6-DMSO at room temperature.

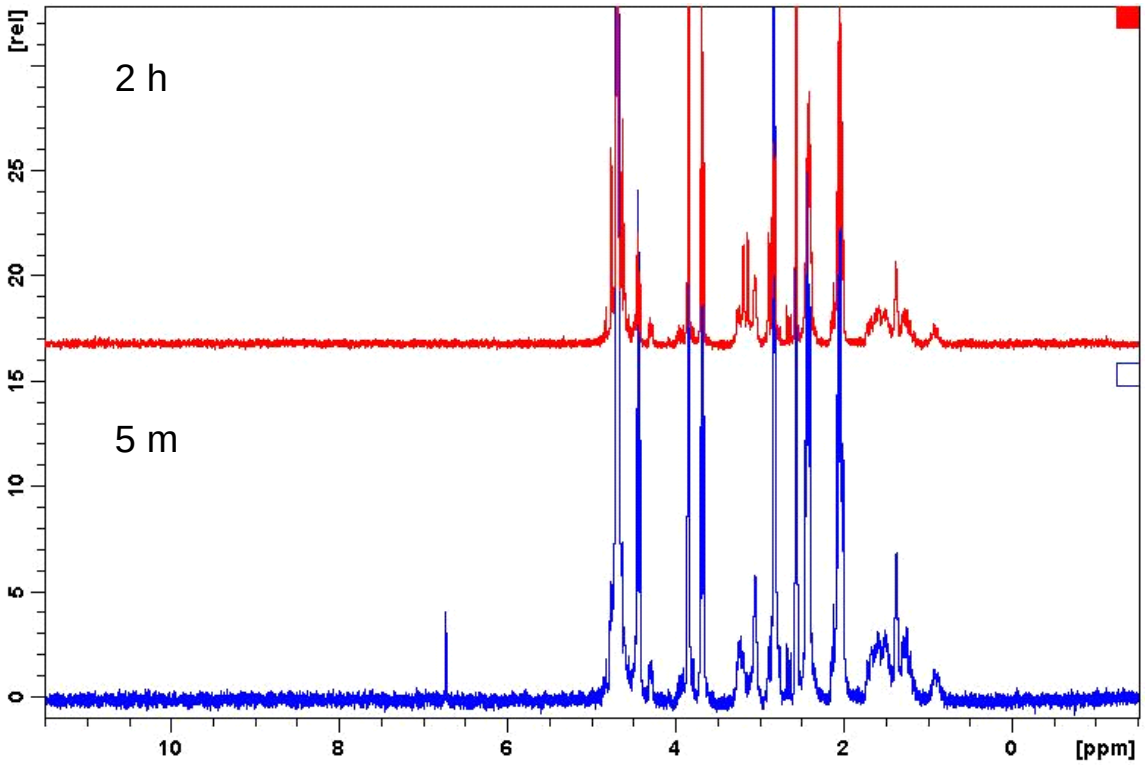

Figure S6. ^{1}H-NMR spectra recording the conversion of BMCC (1 mM) to its GSH conjugate GS-BMCC in D_2O containing 10% d_6-DMSO at room temperature.

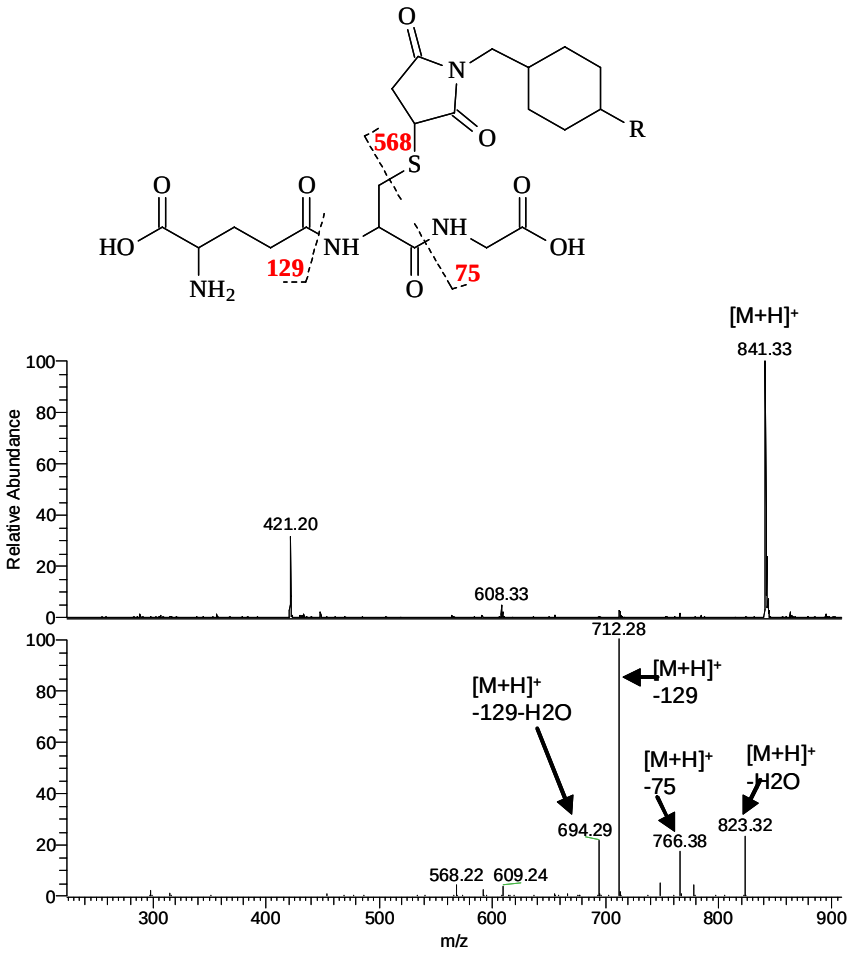

Figure S7. MS-MS of GS-BMCC.

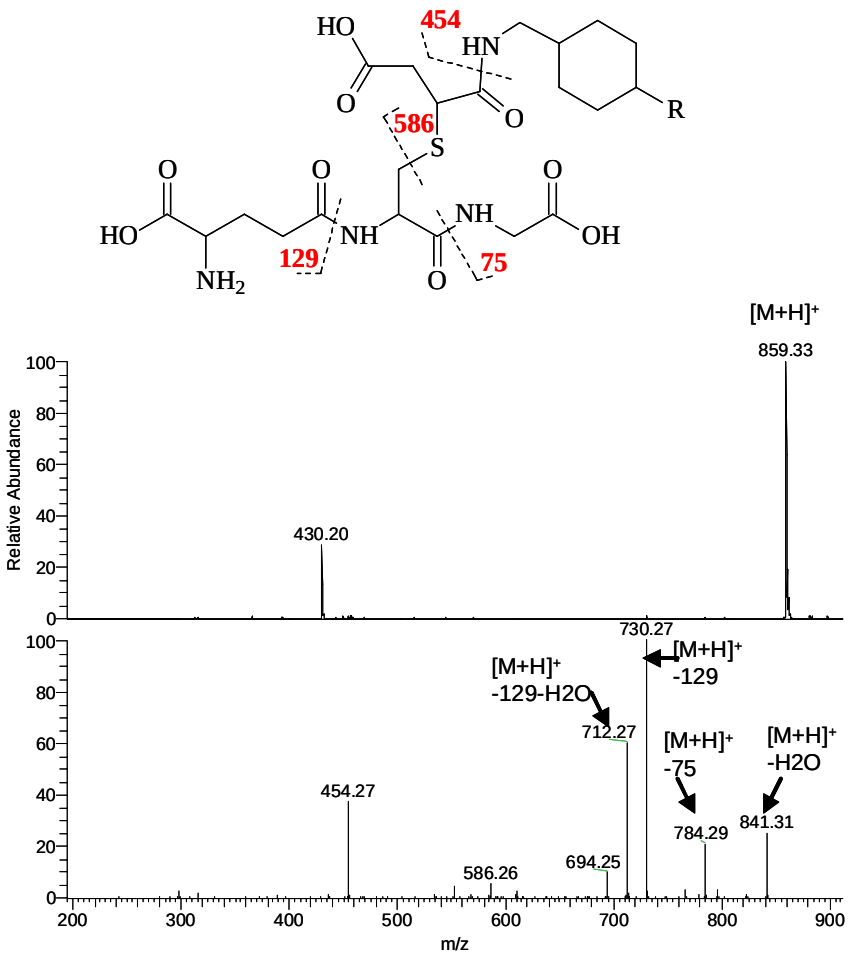

Figure S8. MS-MS of GS-BMCC-acid.